

PB85-173904

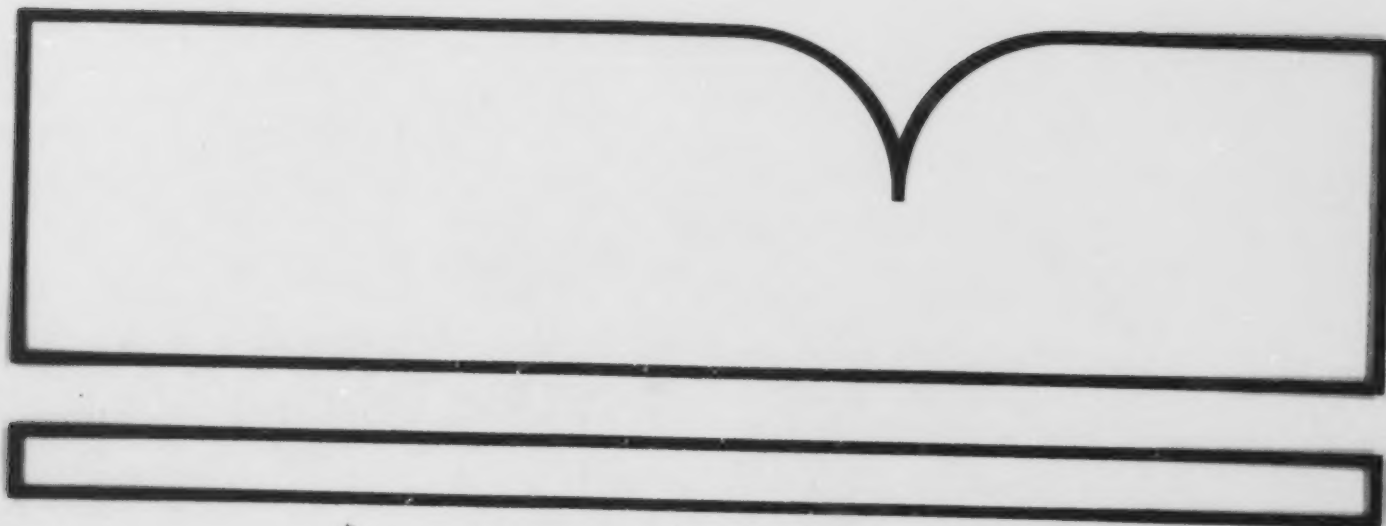
Interim User's Manual for the Advanced
Scavenging Module Version 1.2

Battelle Pacific Northwest Labs., Richland, WA

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Mar 85



U.S. Department of Commerce
National Technical Information Service

NTIS

PB85-173904

EPA/600/8-85/005
March 1985

AN INTERIM USER'S MANUAL FOR
THE ADVANCED SCAVENGING MODULE
VERSION 1.2

by

J. M. Hales
Battelle Northwest Laboratory
Richland, Washington 99352

Interagency Agreement DW89930059

Project Officer

J. L. Durham
Atmospheric Chemistry and Physics Division
Atmospheric Sciences Research Laboratory
Research Triangle Park, North Carolina 27711

ATMOSPHERIC SCIENCES RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
RESEARCH TRIANGLE PARK, NORTH CAROLINA 27711

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA (Please read Instructions on the reverse before completing)		
1. REPORT NO. EPA/600/8-85/005	2.	3. RECIPIENT'S ACCESSION NO. PB85 173904 /AS
4. TITLE AND SUBTITLE AN INTERIM USER'S MANUAL FOR THE ADVANCED SCAVENGING MODULE VERSION 1.2	5. REPORT DATE March 1985	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) J. M. Hales	8. PERFORMING ORGANIZATION REPORT NO.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS Battelle Northwest Laboratory Richland, Washington 99352	10. PROGRAM ELEMENT NO. CCVN1A:04 Task 3100 FY-85	11. CONTRACT/GRANT NO. IAG DW89930059-01-2
12. SPONSORING AGENCY NAME AND ADDRESS Atmospheric Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, North Carolina 27711	13. TYPE OF REPORT AND PERIOD COVERED Interim	14. SPONSORING AGENCY CODE EPA/600/09
15. SUPPLEMENTARY NOTES		
16. ABSTRACT This report provides a user's manual for Version 1.2 of the Advanced Scavenging Module (ASM). It is an interim code and is intended primarily for coordinating development of the module with that of the evolving NCAR Regional Acid Deposition Model (RADM). The ASM is currently in an evolutionary stage ; the general framework provided by Version 1.2 is sufficiently well-established to provide the basis for future versions. The code supplied with this manual is a complete, operational system, and was tested. The ASM is activated by two types of subroutine calls from the host code. Upon advancing to some ground-level position (x,y) on the host's numerical computation grid, the ASM is interrogated (using the first subroutine call) to produce the vertical distributions of storm features above that point. Following this, scavenging computations are performed repeatedly for each vertical grid position, using the second subroutine call. The primary outputs from these secondary ASM interrogations are the transformation rates associated with the physical and chemical components of the scavenging process. These rates are returned to the host code and incorporated with its normal numerical integration procedure.		
17. KEY WORDS AND DOCUMENT ANALYSIS		
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED	21. NO. OF PAGES 65
	20. SECURITY CLASS (This page) UNCLASSIFIED	22. PRICE

NOTICE

The information in this document has been funded by the United States Environmental Protection Agency under Interagency Agreement DW89930059 to Battelle Northwest Laboratories. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document. Mention of trade names or commercial products does not constitute endorsement or recommendation for use.

ABSTRACT

This report provides a user's manual for Version 1.2 of the Advanced Scavenging Module (ASM). Version 1.2 is an interim code, and is intended primarily for coordinating development of the module with that of the evolving NCAR Regional Acid Deposition Model (RADM).

Although the ASM is currently in an evolutionary stage, the general framework provided by Version 1.2 is sufficiently well-established to provide the basis for all future versions. The code supplied with this manual is a complete, operational system, and can be executed with the RADM or other "host" codes for extensive development and testing.

The ASM is activated by two types of subroutine calls from the host code. Upon advancing to some ground-level position (x,y) on the host's numerical computation grid, the ASM is interrogated (using the first subroutine call) to produce the vertical distributions of storm features above that point. Following this, scavenging computations are performed repeatedly for each vertical grid position, using the second subroutine call. The primary outputs from these secondary ASM interrogations are the transformation rates associated with the physical and chemical components of the scavenging process. These rates are returned to the host code and incorporated with its normal numerical integration procedure.

Future versions of the ASM will contain much more complete depictions of storm features and associated phenomena. Several such versions will become available during the next two years.

This report was submitted as a DOE related-services effort under Contract 1830, under the support of the Environmental Protection Agency. This report covers a period of November 30, 1983 through November 30, 1984, and work was completed on November 30, 1984.

CONTENTS

Abstract.	iii
Figures	vi
Tables.	vii
1. Introduction	1
2. Basic Interties with Host Code: Special Forms of Governing Equations	3
3. ASM Functions: A Descriptive Overview	7
4. Operational Overview	16
5. Example Application.	24
References.	36
Appendix	
A. Listing of ASM Version 1.2 Code	37

FIGURES

<u>Number</u>		<u>Page</u>
1	ASM - Host Information Exchange.	8
2	Example Condensed-Water Profiles as Synthesized by the ASM.	.13
3	Schematic of Grid Structure	.17
4	Flow Chart for Subroutine ASM	.18
5	Flow Chart for Subroutine Storm	.20
6	Flow Chart for Subroutine CBCTFL.	.22
7	Interaction Diagram for Sulfur Species.	.31

TABLES

<u>Number</u>		<u>Page</u>
1	Current Empirical Fitting Forms for Snow and Total Precipitation Profiles.	10
2	Current Empirical Fitting Forms for Cloud-Water Profiles.	12
3	Listing of Test Program	25
4	Example Output: Storm Features	27
5	Definition of Variables and Associated Index Names.	29
6	Example Output: WETGEN(IZ,K) for IZ=7.	34

SECTION 1

INTRODUCTION

The Advanced Scavenging Module (ASM) is a conceptual framework and computer code for calculating the precipitation scavenging of reactive and nonreactive air pollutants. The module is intended to be used in conjunction with a regional, Eulerian "host" code, which approximates numerically the appropriate equations of conservation and interrogates the ASM for needed input regarding wet-chemistry and scavenging processes. The ASM can be considered an advancement over its regional predecessors at this point in time, because it is structured to allow a comparatively versatile depiction of individual physicochemical processes within the composite scavenging sequence. This in turn presents the possibility of more accurate source-receptor analysis, and the fruitful investigation of individual chemical contributions, nonlinear effects, and associated control strategies. The ASM is being prepared primarily for the NCAR Regional Acid Deposition Model (RADM) and an enhanced version of the existing STEM II code, but is sufficiently versatile to be incorporated with a number of additional Eulerian models as well.

This version of the module is not submitted as a product that is ready for routine incorporation in a finalized regional model. It is intended, rather, to provide a systematic definition of information-exchange requirements, for the purpose of helping to coordinate development in the overall regional modeling effort. The Version 1.2 Scavenging Module described in this report takes the form of an executable system of subroutines, which may be interrogated by host codes for development and shakedown purposes.

Two coordination points are particularly important in this regard. The first of these is the development of the host-codes, themselves, which must have a number of interactive linkages with the Scavenging Module. The second coordination point is with those individuals who are creating the wet-chemical conversion parameterizations for the RADM. In its present state the Scavenging Module provides a convenient substrate for interweaving these parameterizations with cloud-physics processes and gaseous-phase chemistry. Individuals working on both of these efforts should be totally

aware of the protocols established in the Scavenging Module, so that a smooth coordination of these linkages will occur. In this context it should be noted that while many internal features of the Scavenging Module are not complete, the framework and information-exchange scheme is in a rather high state of development. Because of this, coordination with other modules and with the host codes can occur at this point with minimum fear of future backtracking.

The Advanced Scavenging Module bears a direct relationship with the evolving reactive storm models in the PLUVIUS series, and many of the procedures and parameterizations employed by the Module are directly traceable to those used in the PLUVIUS codes. Two primary differences exist. The first of these is that the Module is subservient to the host code and is designed to work interactively with a number of outside modules, whereas the PLUVIUS models deal with the total system of conservation equations. The second difference is that the PLUVIUS codes generate storm systems on the basis of first principles, whereas the Scavenging Module synthesizes the storms on the basis of empirical formulae and look-up tables. This feature is appropriate to the Module for two major reasons: first, it allows a very rapid and computationally efficient generation of essential properties, and second, it provides a convenient means for creating spatially- and temporally-averaged storm features. This is particularly important for the target models, because of temporal and spatial grid-mesh properties.

The Version 1.2 described in this report has been written in standard FORTRAN 77 code and, other than for architectural features, has not been prepared for vectorization on an array-processor. In particular, many of the innermost loops contain conditional statements, which will prevent direct vectorization. This choice was made with Version 1.2 because the primary objective of this version is to coordinate development and illustrate information exchange, and inclusion of the conditional statements results in a much more easy-to-follow text. A vectorized replica of Version 1.2 will be prepared, for initial blending with the RADM on the NCAR Cray array processor. Upgraded versions of the Advanced Scavenging Module will become available periodically during the next two years.

SECTION 2

BASIC INTERTIES WITH HOST CODE: SPECIAL FORMS OF GOVERNING EQUATIONS

The ASM presumes that the host code's governing equations possess certain well-defined components, and it is important at the outset to describe these essential qualities explicitly. This can be accomplished by deriving a species-conservation equation and identifying pertinent intertie terms. Conservation of species A can be expressed by the basic continuity equation as

$$\frac{\partial C_{Am}}{\partial t} = - \nabla \cdot (C_{Am} \underline{v}_{Am}) + R_{Am} \quad (1)$$

where C_{Am} is the concentration of species A in medium m,* (moles of m-bound A per unit volume total space),

$\underline{v}_{Am}$ is the velocity vector of species A in medium m, and

R_{Am} is a volumetric source-sink term for species A in medium m.

$$\underline{v}_{Am} = \hat{u} \hat{i} + \hat{v} \hat{j} + \hat{w} \hat{k}$$

has several components. In particular, the vertical velocity is composed of

- 1) the vertical air velocity, w;
- 2) the vertical diffusive velocity of species A in medium m; and
- 3) the vertical fall velocity of species A in medium m, w_{Am} .

Thus

$$\hat{w} = w - \frac{C}{C_{Am}} K_{zm} \frac{\partial r_{Am}}{\partial z} + w_{Am} \quad (2)$$

*The word "medium" pertains to air, rain, snow, ..., i.e., whatever phase in which the species resides.

where c is the molar concentration of air molecules,

K_{zm} is the effective vertical diffusivity of medium m , and

r_{Am} is the mixing ratio of species A in medium m (moles of m -bound A per mole of air) (c_{Am}/c)

Combination of Equations (1) and (2) gives

$$\frac{\partial c_{Am}}{\partial t} = -\nabla \cdot (c_{Am} \mathbf{v}) + \nabla \cdot \mathbf{K}_{zm} \cdot \nabla r_{Am} - \frac{\partial}{\partial z} (c_{Am} w_{Am}) + R_{Am} \quad , \quad (3)$$

where $\mathbf{v}$ is the wind-velocity vector, and

$\mathbf{K}_{zm}$ is the diffusivity tensor corresponding to medium m .

Equation (3) assumes that horizontal transport properties (velocities, diffusivities) are the same for all species and all media.

Applying the mass-continuity equation to (3) and expressing the dependent variable as a mixing ratio gives

$$\rho \frac{\partial r_{Am}}{\partial t} = -\rho \nabla \cdot r_{Am} \mathbf{v} - \frac{\partial}{\partial z} (\rho r_{Am} w_{Am}) + \nabla \cdot \rho \mathbf{K}_{zm} \cdot \nabla r_{Am} + M_A R_{Am} \quad (4)$$

where ρ is the air density and M_A is the molecular weight of air. This may be transformed to an alternate vertical coordinate system (e.g., a σ system), if desired.

Equation (4) is typical of the species-conservation equations employed by most comprehensive air-pollution models, with two important exceptions:

1. It contains the vertical fall-velocity term $\frac{\partial}{\partial z} (\rho r_{Am} w_{Am})$. This term is essential to scavenging calculations because of vertical transport by precipitation.*
2. The z-component of the diffusivity tensor can vary from one medium (air, rain, ...) to the next. This can be important because of pseudo diffusion caused by differential settling of various sizes of hydrometeors.

The above two features summarize special requirements imposed on the host-code governing equations by the ASM. In addition to this, the lower boundary conditions of the host code require somewhat special treatment:

3. The lower boundary conditions of the host code must be sufficiently flexible to accommodate "outflow" type boundary conditions when demanded by falling precipitation.

All of these special requirements can be incorporated easily into the RADM. This should be done at the outset of the code's development, however, to avoid costly retrofitting downstream.

The ASM is designed to interact with the host code by supplying to Equation (4) (or some logical counterpart) values of w_{Am} , K_{zm} , and R_{Am} .[†] To accomplish this the host code must supply to the ASM values of r_{Am} and a

*It should be noted here that inclusion of vertical fall velocity will increase the magnitude of the vertical Courant number

$$N_{cz} = \frac{(w + w_{Am}) \Delta t}{\Delta z} ;$$

Δt = advection time step in numerical computation;

Δz = vertical grid spacing in numerical computation;

This is an important factor influencing the computational performance of most numerical integration techniques.

[†]It should be noted here that R_{Am} includes not only chemical conversion, but physical modification and interphase transport as well. The ASM is designed to provide only the wet-chemical and physical-interchange components of R_{Am} . Homogeneous gas-phase conversion rates are presumed to be generated elsewhere in the host code.

number of "predictor variables." This intertie is shown schematically in Figure 1. All of these variables are presumed to be exchanged via program COMMON, leaving subroutine call argument lists open primarily for control parameters.

SECTION 3

ASM FUNCTIONS: A DESCRIPTIVE OVERVIEW

The ASM operates in two distinct modes, which may be termed the "storm-generation" and "scavenging" modes. Activation of these modes is controlled via a subroutine argument (MFUNCT), and a number of internal bypass options are available, depending on specific computations required by the particular host code in use.

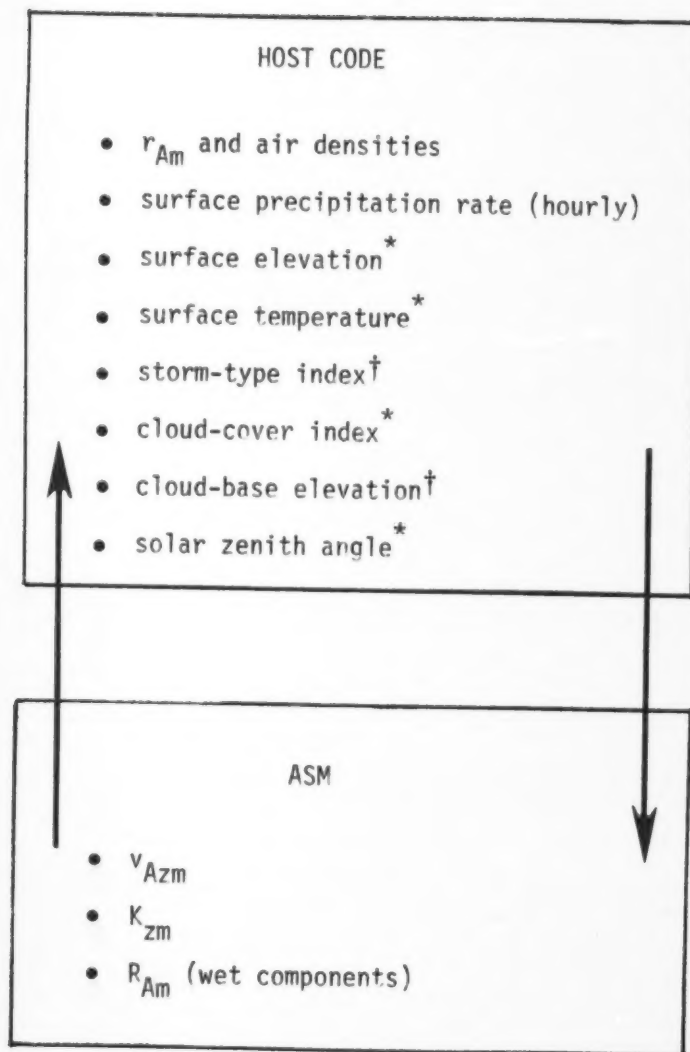
In storm-generation mode, the ASM creates vertical profiles of key storm parameters above some chosen position x,y at the surface. These parameters include quantities of the condensed-water media and their associated interconversion rates, as well as a number of auxiliary variables (such as actinic flux) required for reactive scavenging calculations. Condensed-water media for this particular version of the ASM have been lumped into the three following categories:

- cloud water,
- rain,
- snow.

These categories were chosen primarily on the basis of experience with diagnostic storm models, which have demonstrated this type of lumping to provide a reasonable balance between simplicity and reality. Depending on initial experience with the ASM--host-code merger, however, this categorization may be modified in future versions.

Vertical profiles of these condensed-water classes are estimated using empirical relationships. ASM version 1.2 employs polynomial fitting functions for this purpose, in conjunction with the following "predictor variables", which are presumed to be supplied from the host code (cf. Figure 1):

- surface precipitation rate,
- surface elevation,
- surface temperature,
- storm-type index,
- cloud-cover index,
- cloud base elevation.



* Required only in "storm-generation" mode.

† Redundant and will be consolidated at a later date.
Provision should be made for incorporation, however.

Figure 1. ASM - Host Information Exchange

Forms of version 1.2's polynomial fitting functions are summarized in Tables 1 and 2, and example profiles are shown in Figure 2. It is important to note that Table 1's equations for precipitation are based on precipitation fluxes, rather than concentrations. During the code's operation, the fluxes are computed using the noted relationships, with subsequent determination of the associated concentrations via division by the appropriate vertical velocities. Polynomials are employed for "snow" and "total precipitation", and "rain" is determined as the difference between these two.

There are a number of noteworthy features of this procedure.

- The "predictor variables" itemized above are not unique, and should be considered as tentative. Their choice is dictated primarily by their sensitivity and specificity as predictors of storm features and by the reasonable prospect of their availability within the host code. Moreover, there is considerable redundancy in the listing shown here, and future consolidation can be anticipated.
- The forms of the fitting functions may be subject to future change. This will depend on the adequacy of the present forms to depict desired storm behavior, as operating experience is gained with the module.
- Some host codes may include internal generation of cloud and precipitation profiles. In this event, the above calculations are immaterial. The ASM provides a bypass option for this situation.

In addition, it should be noted that one could have employed a deterministic model, rather than empirical functions, within the ASM to generate vertical precipitation and cloud profiles. The empirical alternative was chosen here for two primary reasons. The first of these is that empirical relationships provide considerably more computational economy than do their more deterministic counterparts. This is an important factor in most regional-modeling operations, owing to their computationally intensive nature. The second factor favoring empirical depiction is the desirability

TABLE 1. CURRENT EMPIRICAL FITTING FORMS FOR SNOW
AND TOTAL PRECIPITATION PROFILES

CASE 1: Cloud Base Below Freezing Level		
Zone	Snow	Total Precipitation
<u>Zone I</u>		
CT>Z>FL	$DS31 \left[0.5(CT-CB)^3 - 1.5(CT-CB) \right. \\ \left. (Z-CB)^2 + (Z-CB)^3 \right]$	
<u>Zone II</u>		
FL>Z	$DS31 \left[0.5(CT-CB)^3 - 1.5(CT-CB) \right. \\ \left. (FL-CB)^2 + (FL-CB)^3 \right] + CS21 \\ (Z-FL)^2$	
<u>Zone III</u>		
CT>Z>CB		$DP31 \left[0.5(CT-CB)^3 - 1.5(CT-CB) \right. \\ \left. (Z-CB)^2 + (Z-CB)^3 \right]$
<u>Zone IV</u>		
CB>Z		$0.5 DP31 (CT-CB)^3 + CP21 \\ (Z-CB)^2$

TABLE 1 (continued)

CASE 2: Cloud Base Above Freezing Level

Zone	Snow	Total Precipitation
<u>Zone I</u>		
Cloud Top > Z > Cloud Base	$DS32 \left[0.5(CT-CB)^3 - 1.5(CT-CB)(Z-CB)^2 + (Z-CB)^3 \right]$	$DS32 \left[0.5(CT-CB)^3 - 1.5(CT-CB)(Z-CB)^2 + (Z-CB)^3 \right]$
<u>Zone II</u>		
Cloud Base > Z > Freezing Level	$0.5 DS32 (CT-CB)^3 + BS12 (Z-CB)$	$0.5 DS32 (CT-CB)^3 + BS12 (Z-CB)$
<u>Zone III</u>		
Freezing Level < Z	$0.5 DS32 (CT-CB)^3 + BS12 (FL-CB) + CS22 (Z-FL)^2$	$0.5 DS32 (CT-CB)^3 + BS12 (FL-CB) + CP22 (Z-FL)^2$

* CB = Cloud Base Elevation

CT = Cloud Top Elevation

FL = Freezing Level

Z = Elevation

All other terms are empirical coefficients

TABLE 2. CURRENT EMPIRICAL FITTING FORMS
FOR CLOUD-WATER PROFILES

CLOUD WATER CONCENTRATION =

$$A + B (Z-CB) + C(Z-CB)^2 + D (Z-CB)^3$$

Where:

$$A = C_0$$

$$B = D_0$$

$$C = - \frac{3 C_0 + 2 D_0 (CT-CB)}{(CT-CB)^2}$$

$$D = \frac{2 C_0 + D_0 (CT-CB)}{(CT-CB)^3}$$

NOTE: C_0 and D_0 are the stipulated cloud-water concentration and derivative of cloud-water concentration with respect to height, respectively, at cloud base. These are empirical parameters of the distribution.

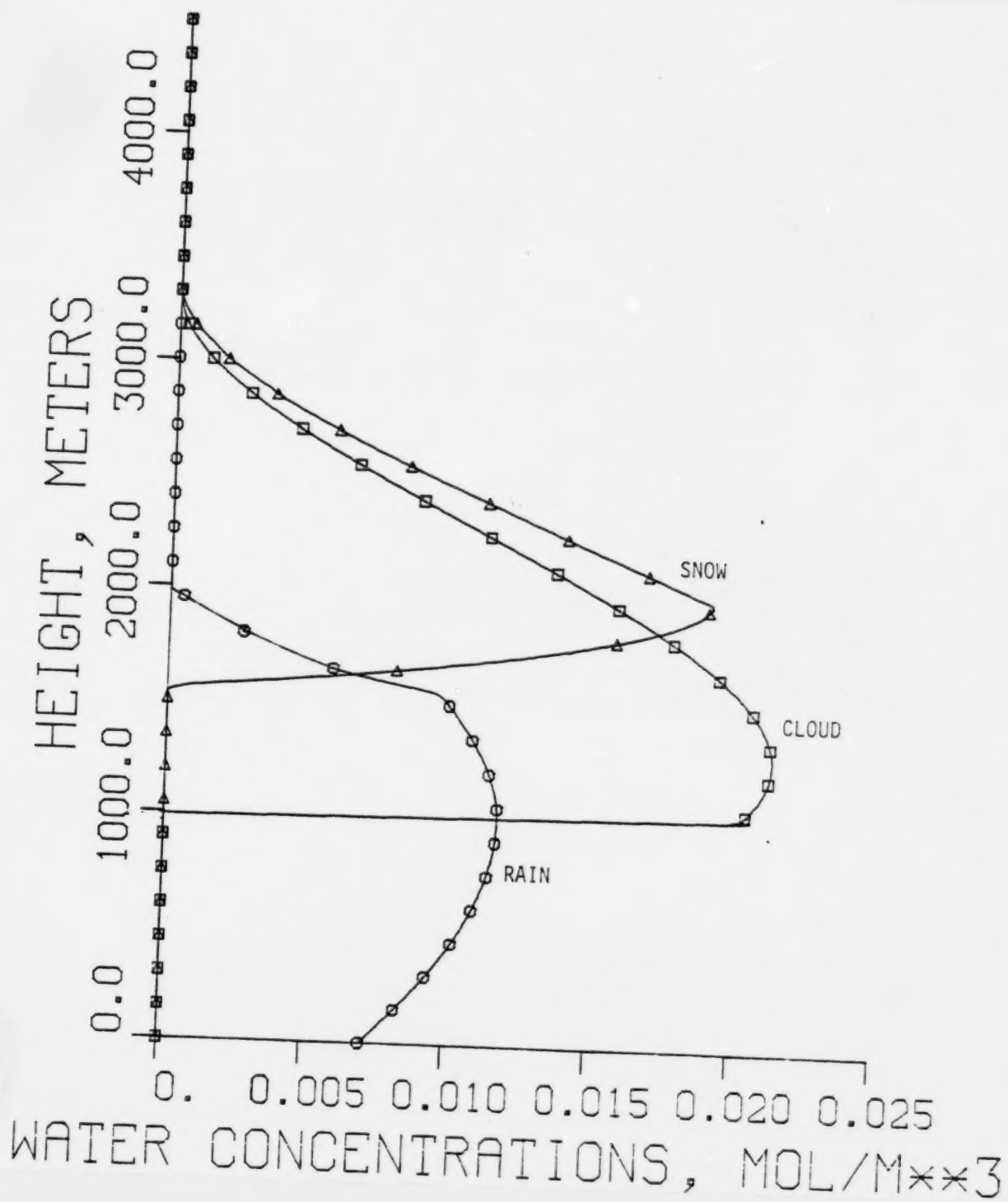


Figure 2. Example Condensed-Water Profiles as Synthesized by the ASM

of employing storms which represent spatially-, temporally-, or even climatologically-averaged conditions. This is virtually impossible with deterministic storm models. While the problem of just how to characterize such "average" storms appropriately is by no means trivial, this process can be implemented in principle, at least, in a direct manner using empirical relationships.

Cloud interconversion processes of potential importance to the scavenging process include

- cloud autoconversion to rain,
- accretion of cloud water by rain,
- riming of cloud water by snow,
- deposition of water vapor to snow surfaces,
- freezing of liquid water,
- melting of snow, and
- evaporation of condensed water.

Transport processes included by the storm environment include

- vertical fall velocities of snow and rain, and
- dispersion of snow and rain arising from differential settling of different sizes of hydrometeors.

All of these properties are computed by the ASM in storm-generation mode. The code is modularized to accommodate progressive improvements in characterizations of these features, and the present Version 1.2 employs the rather simple expressions utilized by the PLUVIUS MOD 5.0 storm code (Easter and Hales, 1984). Since these expressions are described in the PLUVIUS user's manual, they will not be discussed at length in the present document.

It should be noted that the transport properties v_{Azm} and K_{zm} generated within this portion of the ASM are important outputs to be employed by the host code [cf. Figure 1 and Equation 4]. All other features calculated within the storm-generation mode are intended for subsequent use by the ASM in its "scavenging" mode, where the sole output product is the vector of physicochemical "wet" conversion rates, WETGEN(K). One should note here that the ASM is interrogated once per advection time-step in storm-generation mode at each value of x, y . Typically, however, it will be

interrogated numerous times in scavenging mode, since reaction computations must be performed at each vertical position and at several sub-increments of time. In this context the ASM presupposes that the host code contains a component which numerically integrates the physicochemical conversion equations using the following process:

- step to point z, t (at some predetermined position x, y),
- interrogate the host code's air-chemistry subroutine to obtain DRYGEN(K), the vector of homogeneous conversion rates at location z ,
- interrogate the ASM in scavenging mode to obtain corresponding values of WETGEN(K),
- add corresponding elements of WETGEN and DRYGEN to obtain the composite physicochemical conversion rates, R_{Am} ($A_m \equiv K =$ species/medium index),
- apply these composite rates in conjunction with the host's ordinary differential-equation integration scheme to determine the dependent variables [r_{Am} in Equation 4] at time $t + \delta t$.

Formulation of physicochemical relationships within the ASM's scavenging mode can be best illustrated by means of an example. Suppose that one of the dependent variables in the vector r_{Am} pertained to the mixing ratio of rainborne sulfate. Conceivably this material can be generated by the following processes:

- melting of sulfate-containing snow,
- accretion and autoconversion of sulfate-containing cloud water,
- oxidation of rainborne SO_2 ,
- capture of sulfate aerosol.

Corresponding loss terms are

- freezing of sulfate containing rain.

To formulate an appropriate rate expression one simply adds these contributions and expresses the result at the appropriate location in the ASM. This is precisely the procedure employed within the PLUVIUS storm code, and is illustrated further by the example discussed in the final section.

SECTION 4

OPERATIONAL OVERVIEW

The ASM can be considered to be quasi one-dimensional in the sense that, at any given point in time, it considers only those scavenging processes occurring within a vertical column of air above some surface point (x,y).^{*} This can be illustrated by considering Figure 3, which is a segment of the numerical grid within the host code. Let us suppose that the host code has progressed in its numerical integration scheme to the point (x,y), and is now ready to perform computations in the vertical direction for the grid points z(1), z(2), ..., z(nz). The first scavenging-module interrogation must occur at this point, using the call

CALL ASM(IX,IY,IZ,1,ITOGGL)

where IX, IY and IZ are the grid indices, the argument 1 (MFUNCT) specifies that the module is in "storm-generation" mode, and ITOGGL is a "storm toggle" to be described below.

As indicated by the flow diagram in Figure 4, the first operation in storm-generation mode is creation of the internal concentration matrix C(IZ,K) from the four-dimensional mixing-ratio matrix R(IX,IY,IZ,K) employed by the host. This operation is performed for all K=1, ..., NTOT species-medium combinations, including those variables which are computed as steady states; i.e.,

$$\begin{aligned} \text{NTOT} &= \text{NCOMP} + \text{NCNSTR} \\ &= \text{number of "computed" or ordinary dependent variables} \\ &\quad + \\ &\quad \text{number of "constrained" variables (steady states).} \end{aligned}$$

^{*}Storms covering multiple, adjacent grid points can be accommodated in a natural way, simply by proceeding with the point computations in sequence. The discussion here will continue to focus on a single x,y grid point for simplicity.

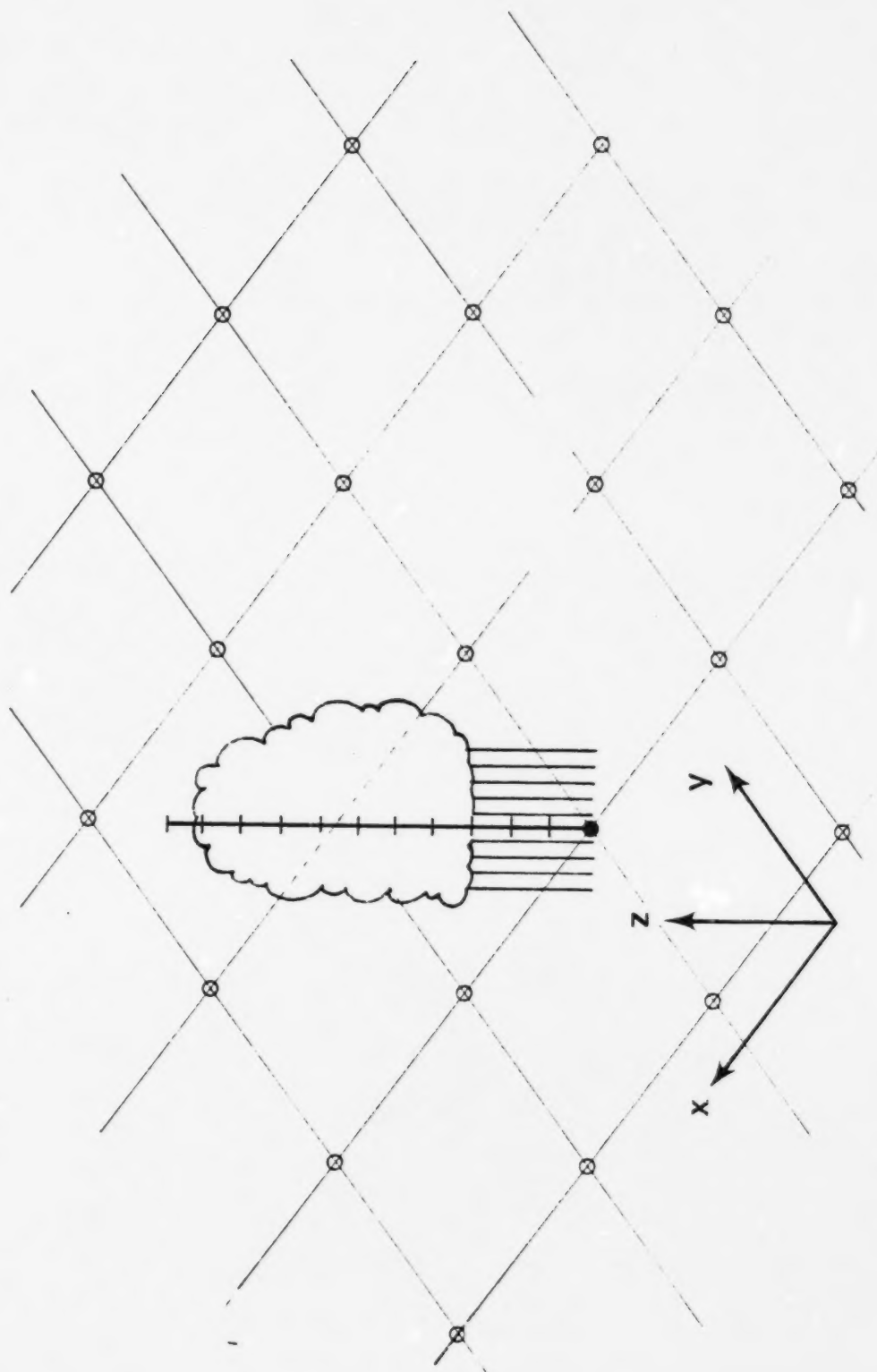


Figure 3. Schematic of Grid Structure

SUBROUTINE ASM (IZ,MFUNCT,ITOGGL)

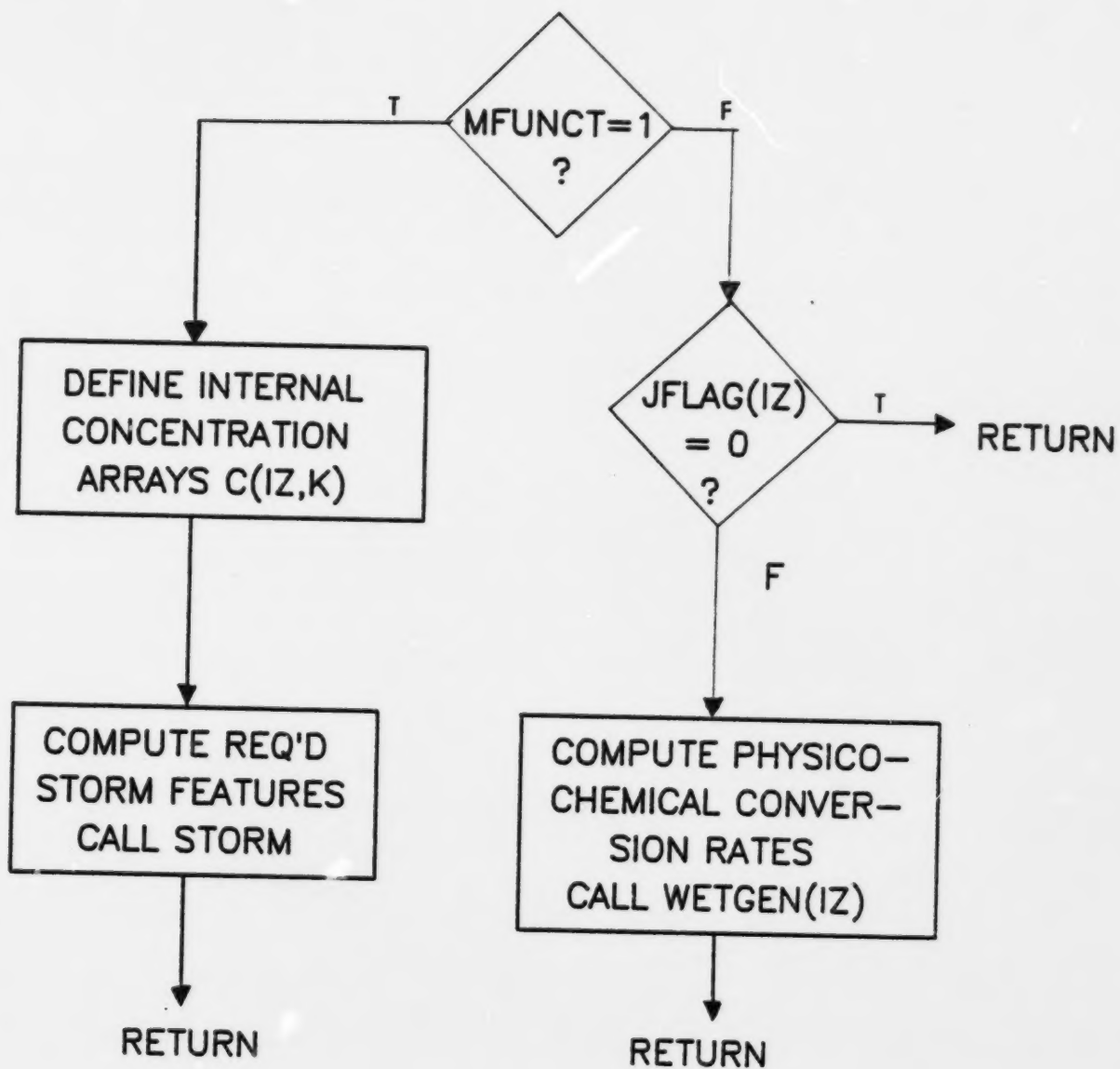


Figure 4. Flow Chart for Subroutine ASM

As noted previously, $R(IX,IY,IZ,K)$ is assumed available to the module via COMMON storage. It is important to re-emphasize at this point that the current ASM version presumes that only three classes of condensed water exist: "cloud", "rain", and "snow". Because of this, four different media are available for the chemical species, and in general one must include a dependent variable R for every species-medium combination.* Thus, for example, four sulfate mixing ratios must be described:

$R(IX,IY,IZ,KS04A),$
 $R(IX,IY,IZ,KS04C),$
 $R(IX,IY,IZ,KS04R),$
 $R(IX,IY,IZ,KS04S).$

where the indices KS04A, KS04C, KS04R, and KS04S pertain to sulfate in aerosol form, in cloud water, in rain, and in snow, respectively.

Following unit conversion the module interrogates the STORM subroutine, as shown in Figure 5. STORM's first function is to examine the bypass variable ITOGGL, which permits short-circuiting of the storm-generation subroutines in the case of pre-existing storm data. This option is of possible importance to the NCAR RADM code, which may apply external dynamic-model calculations to generate storm features. If this is indeed the case, then the system executes subroutine CLEANUP, which essentially corrects-out residual values of $C(IZ,K)$ from pre-existing cloud systems, and exits from the module. In this process, CLEANUP also sets the local condensed-water flag vector JFLAG(IZ) $IZ=1,...,NZ$. JFLAG(IZ) is set equal to zero if no condensed water (cloud, rain, or snow) exists at point IZ. If condensed water does exist, JFLAG(IZ) is set equal to 1.

In the event that $ITOGGL \neq 1$, subroutine STORM proceeds to "generate" storm properties, giving at each vertical grid point the following features:

- concentrations of snow, rain, and cloud water (moles water/m³ air),
- vertical velocities of air, snow, and rain (m/sec),
- actinic flux,

*Obviously, aqueous-medium concentrations do not have to be defined for highly insoluble gases, such as ethylene.

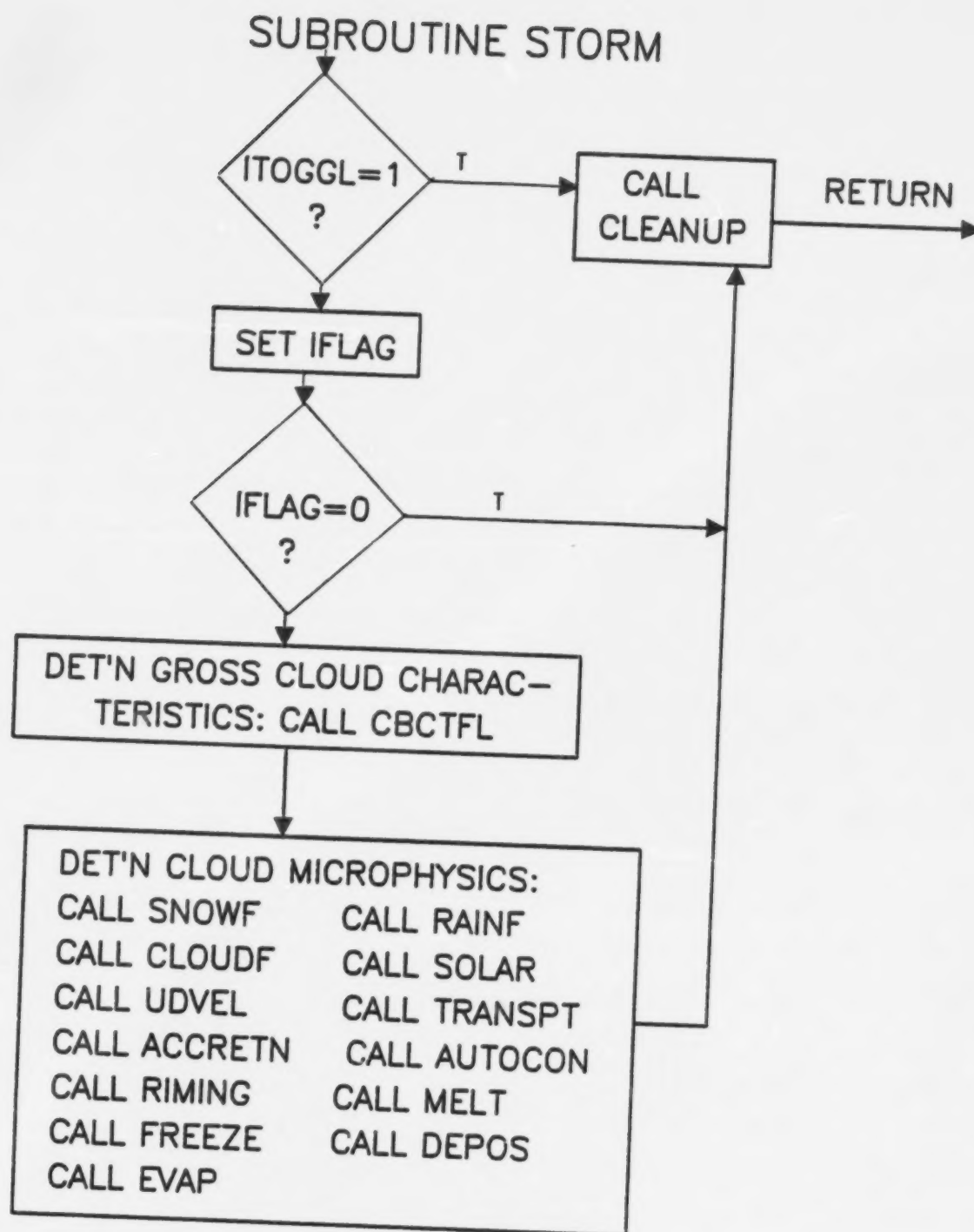


Figure 5. Flow Chart for Subroutine Storm

- cloud-physics interconversion rates or pseudo first-order rate coefficients: autoconversion, accretion, riming, melting, freezing, vapor sublimation, and rain evaporation.

In addition, subroutine STORM sets a global cloud-cover flag, which is defined as

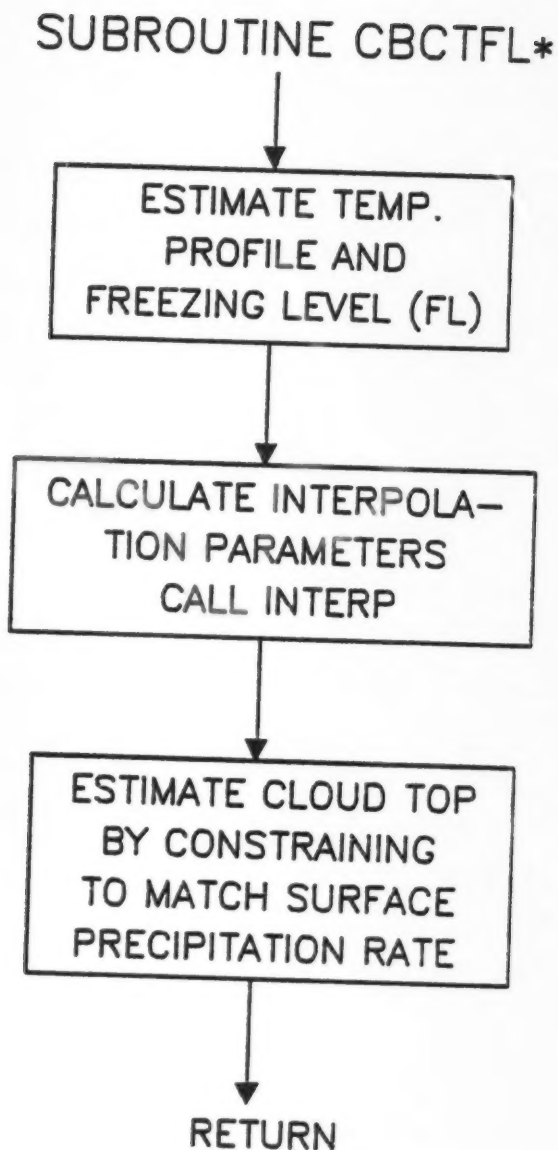
IFLAG = 0 - clear skies
 = 1 - nonprecipitating clouds
 = 2 - surface precipitation.

If a no-cloud (IFLAG=0) condition is detected by subroutine STORM, then a normal exit is performed, subsequent to an interrogation of the CLEANUP routine. In situations where clouds do, indeed, occur, the module proceeds to execute subroutine CBCTFL (Figure 6), which returns elevations of the cloud base (CB),* cloud top (CT), and freezing level (FL). Just how these features will be treated ultimately will depend upon the results of further experimentation, and the module's present architecture has been designed with sufficient versatility to facilitate these changes as they occur.

Upon exiting from subroutine CBCTFL, the code proceeds to compute vertical profiles of the following features, utilizing the obvious subroutine calls:

- snow concentrations (moles water/m³),
- rainwater concentrations (moles water/m³),
- cloudwater concentrations (moles water/m³),
- air vertical velocity (m/sec),
- snow fall velocity (m/sec),
- rain fall velocity (m/sec),
- solar actinic flux (Einsteins/m²sec),
- cloudwater autoconversion rate coefficient (sec⁻¹),
- rain accretion rate coefficient (sec⁻¹),
- snow riming rate coefficient (sec⁻¹),
- snow melting rate coefficient (sec⁻¹),

*Currently CB is supplied as input data.



*CLOUD-BASE ELEVATION ASSUMED AS INPUT DATA
IN VERSION 1,2

Figure 6. Flow Chart for Subroutine CBCTFL

- liquid-water freezing rate coefficient (sec^{-1}),
- vapor deposition rate (to ice) ($\text{moles water/m}^3 \text{ sec}$),
- rain evaporation rate ($\text{moles water/m}^3 \text{ sec}$).

Upon exiting these subroutines, the module executes subroutine CLEANUP and returns control to the host code.

All subsequent calls to the ASM for the current x,y position take the form

```
CALL ASM(IX,IY,IZ,2,ITOGGL) .
```

These calls are expected to appear in the host code's subroutine for integrating the chemical-kinetics systems, which is anticipated to be some type of suitable routine for integrating coupled systems of stiff ordinary differential equations.

The chosen ODE subroutine is expected to be used for computing both aqueous-phase and dry chemical reactions, and is anticipated to require both dry and aqueous reaction-rates at various time substeps within a normal time increment. This will be performed by interrogating a dry reaction-rate subroutine (to be supplied in a separate module) and then by interrogation of ASM using the above call.

Upon any call to subroutine ASM with MFUNCT=2, the code first checks JFLAG(IZ) to determine if aqueous phases are present at position IZ. If not, the subroutine executes an immediate return. When aqueous phase is indeed present (JFLAG $\neq$ 0) then subroutine WETCON is interrogated to produce values of WETGEN for return to the integration scheme. It should be noted here that, although subroutine WETCON appears within the general ASM architecture, this component will be created largely by others working on the RADM effort. It is important to locate WETCON in this manner, however, owing to this subroutine's dependence on data generated by subroutines SNOW, RAIN, CLOUD, SOLAR, AUTO, ... , within the ASM framework.

SECTION 5

EXAMPLE APPLICATION

This final section describes a simple application of the ASM, which is intended to illustrate the module's use and to indicate communication protocols between the module and the host code. As emphasized previously, this version of the ASM and its example applications are NOT intended for purposes other than illustration and initial host-code development. Many features of Version 1.2 have been held in an extremely simple state, to facilitate the illustration of its use. The present example consists of a short computer program which interrogates Version 1.2 of the ASM (listed in the Appendix), printing pertinent results as it proceeds. The first interrogation of the ASM is in "storm-generation" mode and the second is in "scavenging" mode; thus both aspects of the module are illustrated. In a very crude sense, the example computer program can be considered to be a dummy host code.

As illustrated in Table 3 the dummy code begins by setting the vertical computation grid (16 grid points spaced at 300-meter intervals in this example). It then establishes the surface elevation SURFZ, surface precipitation rate SURFP, and the surface temperature SURFT, along with the cloud-base elevation CB and the storm-type index IST.* Following this a vertical array of air concentrations is generated, and subsequently the system is placed in storm-generation mode (MFUNCT=1), with the storm-bypass switch turned off (ITOGGL =0). The ASM is then interrogated to compute storm features.

Printed results from this example are shown in Table 4, which gives cloud water, rain, and snow as functions of height at each of the grid elements. All of the other pertinent storm features have been computed by this call of the ASM as well, but are not shown here. It is important to note, however, that the total ensemble of these features has been stored in memory at this point, and is available for subsequent use--either by the ASM or by the host code.

*There is only one storm type allowed in the present ASM Version 1.2. This will be expanded in subsequent versions.

TABLE 3. LISTING OF TEST PROGRAM

```

C      INCLUDE 'SCAVCOM.FOR'
C
C      DUMMY PROGRAM FOR ASM TEST
C      FIRST INITIALIZE CONCENTRATION ARRAYS
C
      IX=1
      IY=1
      DO 1 IZ=1,NZ
      R(IX,IY,IZ,KS02AC)=1.E-8
      R(IX,IY,IZ,KS04C)=1.E-9
      R(IX,IY,IZ,KS04R)=1.E-10
      R(IX,IY,IZ,KS02R)=1.E-11
      R(IX,IY,IZ,KS02S)=1.E-11
      R(IX,IY,IZ,KS04S)=1.E-10
      R(IX,IY,IZ,KS04A)=1.E-11
1
C
C      NEXT SET GRID AND PREDICTOR VARIABLES
C
      Z(1)=0.
      DZ=300.
      DO 10 IZ=2,NZ
10     Z(IZ)=Z(IZ-1)+DZ
      SURFZ=Z(1)
      SURFP=.02
      CB=1000.
      SURFT=288.
C
C      NOW CREATE A VERTICAL PROFILE OF AIR CONCENTRATIONS
C      (MOLES/M**3)
C
      CAIR(1)=43.09
      DO 15 IZ=2,NZ
15     CAIR(IZ)=CAIR(1)*EXP(-9.09E-5*Z(IZ))
C
C      DO EXAMPLE COMPUTATION IN STORM-GENERATION MODE
C
      MFUNCT=1
      ITOGGL=0
      CALL ASM(IX,IY,IZ,MFUNCT,ITOGGL)
      DO 20 I=1,NZ
      IZ=NZ+1-I
      WRITE(6,200) Z(IZ),TEMP(IZ),CLOUD(IZ),SNOW(IZ),
      + RAIN(IZ)
200     FORMAT(1H,5(3X,E10.4))
20     CONTINUE
C
C      DO EXAMPLE COMPUTATION IN SCAVENGING MODE, AT GRID POSITION IZ=7

```

TABLE 3 (continued)

C

```
MFUNCT=0.  
IZ=7  
CALL ASM(IX,IY,IZ,MFUNCT,ITOGGL)  
DO 30 K=1,NCOMP  
WRITE(6,300) WETGEN(K)  
300 FORMAT(1H ,E10.4)  
30 CONTINUE  
STOP  
END
```

C

TABLE 4. EXAMPLE OUTPUT: STORM FEATURES

Height Above Surface (m)	Temperature (°K)	CLOUD $\frac{\text{moles}}{\text{m}^3 \text{ space}}$	SNOW $\frac{\text{moles}}{\text{m}^3 \text{ space}}$	RAIN $\frac{\text{moles}}{\text{m}^3 \text{ space}}$
0.4500E+04	0.2575E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.4200E+04	0.2597E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.3900E+04	0.2618E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.3600E+04	0.2639E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.3300E+04	0.2658E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.3000E+04	0.2677E+03	0.0000E+00	0.0000E+00	0.0000E+00
0.2700E+04	0.2695E+03	0.4421E-02	0.1751E-02	0.0000E+00
0.2400E+04	0.2713E+03	0.8823E-02	0.5738E-02	0.0000E+00
0.2100E+04	0.2730E+03	0.1355E-01	0.1105E-01	0.0000E+00
0.1800E+04	0.2746E+03	0.1777E-01	0.1675E-01	0.0000E+00
0.1500E+04	0.2762E+03	0.2061E-01	0.7585E-02	0.5705E-02
0.1200E+04	0.2777E+03	0.2123E-01	0.0000E+00	0.8340E-02
0.9000E+03	0.2792E+03	0.0000E+00	0.0000E+00	0.9513E-02
0.6000E+03	0.2821E+03	0.0000E+00	0.0000E+00	0.9732E-02
0.3000E+03	0.2851E+03	0.0000E+00	0.0000E+00	0.9137E-02
0.0000E+00	0.2880E+03	0.0000E+00	0.0000E+00	0.7876E-02
			0.0000E+00	0.6045E-02

The physicochemical example treated by the ASM in its second, "scavenging mode" interrogation requires some explanation at this point. It involves the scavenging of SO_2 gas and sulfate aerosol by physical-uptake processes and, in addition, provides for wet oxidation by both H_2O_2 and ozone. The interaction diagram shown in Figure 6 provides a schematic summary of this model system.

There are numerous simplifications in this example, which can be modified or removed as desired by the user. H_2O_2 and ozone concentrations are presumed to remain fixed in time. SO_2 solubility is assumed to be constant. Cloud and rain acidity (which affect the ozone-oxidation process) are expressed by a simple semiempirical function. These and a number of additional constraints allow the computed and constrained variables to be consolidated as shown in Table 5. Seven computed variables appear in this table, indicating that an actual host code would be responsible for approximating seven simultaneous equations of the form Equation (4). The remaining four constrained or "steady-state" variables do not require solution of Equation (4), but must be carried in the computation for the purpose of assisting other calculations. The "index names" appearing in Table 5 are employed by the code to flag the physical significances of the various computed and constrained variables. These are mainly for programming convenience, and are set by a PARAMETER statement within the ASM.

TABLE 5. DEFINITION OF VARIABLES AND
ASSOCIATED INDEX NAMES

<u>Computed Variables</u>	<u>Index Name</u>
sulfate aerosol	KS04A
sulfate in cloud water	KS04C
sulfate in rain	KS04R
sulfate in snow	KS04S
SO ₂ in air and cloud water	KS02AC
SO ₂ in rain	KS02R
SO ₂ in snow	KS02S
<u>Constrained Variables</u>	<u>Index Name</u>
SO ₂ in air	KS02A
SO ₂ in cloud water	KS02C
ozone in air	K03A
H ₂ O ₂ in air	KH202A

Actual computation of the wet-generation rates occurs in the final portion of the ASM's subroutine WETCON, which is listed in the Appendix. The first statement in this portion, for example, computes WETGEN(KS02AC). This is the rate of wet production of gaseous and cloudborne SO₂ in moles per cubic meter of total space per second and, as indicated in Figure 5, results from

- loss by riming, autoconversion, and accretion of SO₂-laden cloud water, and
- loss by oxidation by oxidation via dissolved ozone (CR03) and H₂O₂ (CRH202).

There is no production of gaseous + cloudborne SO₂ in this example, thus WETGEN(KS02AC) is always negative or zero.

The next FORTRAN statement in this sequence pertains to the generation of cloudborne sulfate ion. This results from

- loss by riming, autoconversion, and accretion of sulfate-laden cloud water,
- gain by ozone- and H₂O₂-oxidation of cloud-borne SO₂, and
- gain by nucleation of sulfate aerosol to form sulfate-laden cloud droplets (RNUCL).

Subsequent FORTRAN statements appear in this sequence as logical results of the interaction diagram, Figure 7.

It is instructive at this point to consider in detail the formulation of the wet-chemical conversion rates, which are expressed immediately above in the WETCON listing. The aqueous-phase oxidation rate of SO_2 resulting from the ozone reaction is given by Penkett et al. (1979) as

$$r = \text{rate of } \text{SO}_2 \text{ oxidation} \left(\frac{\text{moles}}{\text{liter water sec}} \right) = \frac{2.9 \times 10^3}{\sqrt{[\text{H}^+]}} [\text{O}_3] [\text{S}^{\text{IV}}] \quad (5)$$

where the bracketed terms pertain to concentrations in moles per liter of water. Since the ASM deals with concentrations and rates that are expressed on a cubic-meter-of-total-space volumetric basis, this equation must be converted. To accomplish this, one may first convert the molar ozone and S^{IV} concentrations, and the reaction rate, to cubic-meter bases; i.e.,

$$\hat{c}_{\text{O}_3} = [\text{O}_3] (10^3) \frac{\text{moles}}{\text{m}^3 \text{ water}} \quad (6)$$

$$\hat{c}_{\text{S}^{\text{IV}}} = [\text{S}^{\text{IV}}] (10^3) \frac{\text{moles}}{\text{m}^3 \text{ water sec}} \quad (7)$$

$$\hat{r} = r(10^3) \frac{\text{moles}}{\text{m}^3 \text{ water sec}} \quad (8)$$

Upon making the obvious substitutions, Equation (5) becomes

$$\hat{r} \left(\frac{\text{moles}}{\text{m}^3 \text{ water sec}} \right) = \frac{2.9}{\sqrt{[\text{H}^+]}} \hat{c}_{\text{O}_3} \hat{c}_{\text{S}^{\text{IV}}} \quad (9)$$

Ozone is presumed to be at solubility equilibrium between the gaseous and aqueous phases. Because of this, a solubility relationship can be employed to express $\hat{c}_{\text{O}_3}$ in terms of its gaseous-phase counterpart:

$$\hat{c}_{\text{O}_3} = 0.45 \text{ C}(\text{IZ}, \text{K03A}) \frac{\text{moles}}{\text{m}^3 \text{ total space}} \quad (10)$$

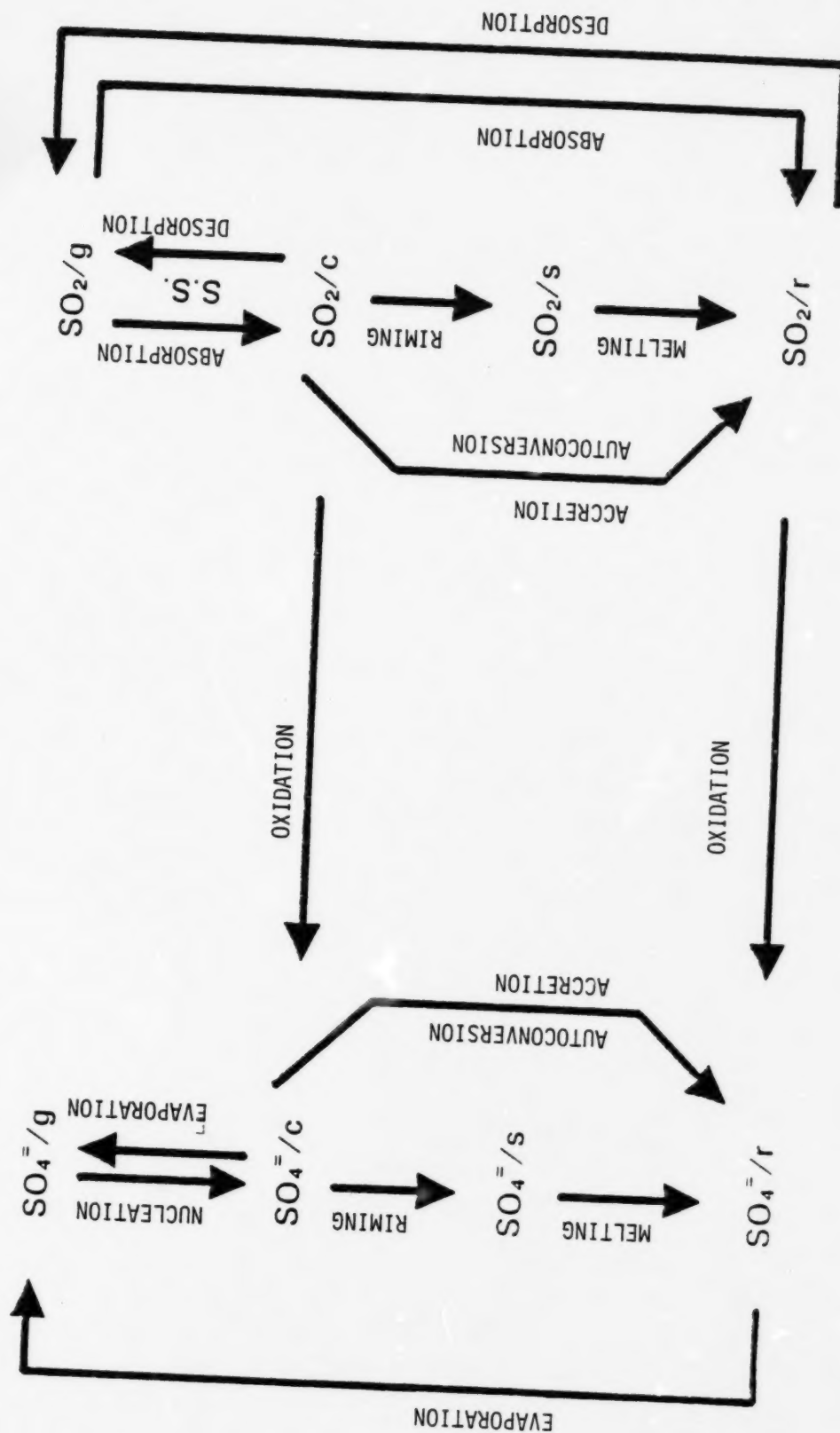


Figure 7. . Interaction Diagram for Sulfur Species

$\hat{r}$ and $\hat{c}_{SIV}$ must be converted to a total-space volumetric basis. This may be done by multiplying by the cloud and rain water volumes:

$$v_{\text{cloud}} = \frac{\text{CLOUD}(\text{IZ}) M_{\text{H}_2\text{O}}}{(\rho_{\text{H}_2\text{O}}) (10)^6} = \frac{\text{CLOUD}(\text{IZ}) (18)}{(1) (10^6)}$$

$$= 1.8 \times 10^{-5} \text{ CLOUD}(\text{IZ}) \frac{\text{m}^3 \text{ cloud water}}{\text{m}^3 \text{ total space}} \quad (11)$$

$$v_{\text{rain}} = 1.8 \times 10^{-5} \text{ RAIN}(\text{IZ}) \frac{\text{m}^3 \text{ rain water}}{\text{m}^3 \text{ total space}} \quad (12)$$

to give the desired rate expressions for cloud and rain water, respectively.

$$\text{CR03} = \frac{1.3}{\sqrt{[\text{H}^+]}} \text{C}(\text{IZ}, \text{K03A}) \text{C}(\text{IZ}, \text{KS02C}) \frac{\text{moles}}{\text{m}^3 \text{ total space sec}} \quad (13)$$

$$\text{RR03} = \frac{1.3}{\sqrt{[\text{H}^+]}} \text{C}(\text{IZ}, \text{K03A}) \text{C}(\text{IZ}, \text{KS02R}) \frac{\text{moles}}{\text{m}^3 \text{ total space sec}} \quad (14)$$

Similar conversions have been performed for the hydrogen peroxide rate expressions, starting from the form

$$r = 8.3 \times 10^{-5} [\text{H}_2\text{O}_2] [\text{undissociated } S^{\text{IV}}] \frac{\text{moles}}{\text{liter water sec}} \quad (15)$$

The reader is encouraged to derive* the coded expressions from this starting point, as a practice exercise.

The primary reason for this detailed presentation of rate-expression conversion is to flag for the reader the importance of the total-space volumetric basis for ASM calculations. Unless one exercises due caution,

*The following approximate values will be helpful for this derivation:
 fraction of dissolved S^{IV} that is undissociated = 0.00925
 solubility of H_2O_2 in water = 10^7

it is extremely easy to confuse units and thus introduce potentially large errors into subsequent calculations.

Two particularly important points should be noted from this discussion. The first of these is that the ASM provides a very natural and realistic technique for "blending" cloud-physics and chemical-conversion processes into a unified description of the reactive cloud environment. The second point is that this modular arrangement makes it convenient to modify descriptions of physicochemical processes. One can, for example, add new chemical species or interaction pathways to the system simply by altering the statements in WETCON and adjusting the dimensioning as appropriate. Used in conjunction with a modern Eulerian host code, this will provide a powerful tool for a variety of applications.

The dummy code in Table 3 activates the scavenging mode of the ASM by setting MFUNCT=1 and defining the vertical grid point at which computations are to proceed. One should note at this point, that computed and constrained variables $R(IX,IY,IZ,K)$ require initialization prior to computation of the generation rates. These were initialized to arbitrarily-chosen values in early statements of the dummy code, and were converted to their corresponding concentrations $C(IZ,K)$ in the storm-generation pass.

Values of WETGEN(K) resulting from the second interrogation of the ASM are shown in Table 6. Nothing is done with these values in the present illustration. In an actual host-code execution, however, these results would be consolidated with corresponding homogeneous, gas-phase conversion rates and employed with an ordinary differential-equation integration scheme to compute updated concentrations, as described on page 15.

There will be some modifications to the ASM which will be necessary for incorporation with individual host codes. Hosts utilizing asymptotic or exponentially assisted ODE solvers will require a segregation of the physicochemical conversion rates into generation and loss terms. This can be accommodated easily by consolidating all positive generation components into the WETGEN array, and defining a new companion array (e.g., WETDEC) for the loss terms. The ASM's structure will also depend to some extent on the PDE numerical scheme of the host. The present version is appropriate for locally one-dimensional schemes such as that employed by STEM. If the

TABLE 6. EXAMPLE OUTPUT: WETGEN(IZ,K) FOR IZ=7

<u>K</u>	<u>Species</u>	<u>WETGEN(IZ,K)</u> <u>g-moles/</u> <u>(m³ total space sec)</u>
1	Sulfate aerosol	-0.6500E-12
2	Sulfate in cloud water	-0.1791E-10
3	Sulfate in rain water	0.4272E-10
4	Sulfate in snow water	-0.1676E-10
5	SO ₂ in air + SO ₂ in cloud water	-0.2277E-11
6	SO ₂ in rain water	0.5252E-10
7	SO ₂ in snow water	-0.1995E-11

RADM scheme evolves as an algorithm having higher local dimensionality, then the dimensioning of the C array in the ASM must be increased as appropriate. This is a relatively minor problem, with the primary drawback of increased memory requirements.

Version 1.2 of the ASM should be considered as a partial guide for host-code development and as a forum for the implementation of wet chemical reaction schemes. The potential user is encouraged to familiarize himself with the ASM by reproducing this example application, and progressively augmenting it as desired. While the ASM's subroutines will undergo extensive development in the future, the framework of the module is essentially at a final stage. Thus it should be relatively easy to incorporate higher versions into existing host codes, once they are formatted to interact with Version 1.2. Several new and improved versions are anticipated during the coming year.

REFERENCES

Easter, R. C. and J. M. Hales. PLUVIUS - A Generalized One-Dimensional Model of Reactant Pollutant Behavior, Including Dry Deposition, Precipitation Formation, and Wet Removal. Pacific Northwest Laboratory, Richland, Washington, 1984.

Penkett, S. A., B. M. R. Jones, K. A. Brice and A. E. J. Eggleton. The Importance of Atmospheric Ozone and Hydrogen Peroxide in Oxidizing Sulphur Dioxide in Cloud and Rainwater. *Atm. Environ.*, 13:123-127, 1979.

APPENDIX A. LISTING OF ASM 1.2 CODE

TABLE A-1. LISTING OF SCAVCOM.FOR

```
PARAMETER (NTOT=11,NCOMP=7,NZ=16,NX=1,NY=1)
PARAMETER (KS04A=1,KS04C=2,KS04R=3,KS04S=4,
+ KS02AC=5,KS02R=6,KS02S=7,KS02A=8,KS02C=9,
+ K03A=10,KH202A=11)
COMMON C(NZ,NTOT),Z(NZ),R(NX,NY,NZ,NTOT),CAIR(NZ),
+ SNOW(NZ),RAIN(NZ),CLOUD(NZ),PRECIP(NZ),VAPOR(NZ),
+ IFLAG,JFLAG(NZ),TEMP(NZ),CS31,DS31,CS21,BS12,CP31,
+ DP31,CP21,BP22,DRAIN(NZ),DSNOW(NZ),RVEL(NZ),SVEL(NZ),
+ AUTO(NZ),ACCR(NZ),RIM(NZ),DEPO(NZ),SMEL(NZ),CO,DO,
+ FREEZ(NZ),EVAP(NZ),ICC,CB,CT,FL,IST,SURFP,SURFT,SURFZ,
+ WETGEN(NCOMP),RNUCL
```

U

TABLE A-2 (continued)

```

      IF(MFUNCT.EQ.1) THEN
C
C      LOAD CONCENTRATION ARRAYS
C
      DO 10 ICOMP=1,NTOT
      DO 10 IZ=1,NZ
10    C(IZ,ICOMP)=CAIR(IZ)*R(IX,IY,IZ,ICOMP)
      CALL STORM(ITOGGL)
      ELSE
C
C      BRANCH FOR WET-CHEMISTRY CALCULATIONS AT POINT IZ
C
      CALL WETCON(IZ)
      ENDIF
      RETURN
      END
C
      SUBROUTINE STORM(ITOGGL)
      INCLUDE 'SCAVCOM.FOR'
C
C      STORM-GENERATION SUBROUTINE: COMPUTES PROFILES OF
C      CONDENSED-WATER CLASSES PLUS PROFILES OF ASSOCIATED
C      INTERCONVERSION RATES AND VERTICAL SETTELING VELOCITIES.
C
      EXIT FOR EXTERNALLY-DEFINED STORM
C
      IF(ITOGGL.EQ.1) THEN
      CALL CLEANUP
      RETURN
      ENDIF
C
C      NOW SET IFLAG
C
      IFLAG=1
      IF(SURFP.GT.0) THEN
      IFLAG=2
      ELSE
      CALL COVER
      IF(ICC.EQ.0.) THEN
      IFLAG=0
      CALL CLEANUP
      RETURN
      ENDIF
      ENDIF
C
C      NOW DETERMINE CLOUD BASE (CB), FREEZING LEVEL (FL), AND
C      CLOUD TOP (CT) (CENTIMETERS)
C
      CALL CBCTFL
C
C      FINALLY INTERROGATE SUBROUTINES TO OBTAIN PERTINENT
C      PROFILES.

```

TABLE A-2 (continued)

```

CALL SNOWF
CALL RAINF
CALL CLOUDF
CALL UDVEL
CALL SOLAR
CALL TRNSPT
CALL AUTOCON
CALL ACCRET
CALL RIMING
CALL MELT
CALL FREEZE
CALL DEPOS
CALL EVAPOR
RETURN
END

```

C

```

SUBROUTINE WETCON(IZ)
INCLUDE 'SCAVCOM.FOR'

```

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

C

THE FOLLOWING CALCULATIONS ARE FOR ILLUSTRATIVE PURPOSES ONLY, AND ARE INTENDED TO DEMONSTRATE THE PROCEDURE FOR LINKING CLOUD PHYSICS, AND WET AND DRY CHEMISTRY TO INTERACT WITH THE COMPOSITE CODE. SOME VERY GROSS SIMPLIFICATIONS HAVE BEEN MADE TO ALLOW A PRIMARY FOCUS ON KEY POINTS. THESE SIMPLIFICATIONS WILL BE REMOVED PROGRESSIVELY AS THE ASM EVOLVES.

THE SCHEME ENVISIONED FOR THIS EXAMPLE IS ONE IN WHICH SO₄ AEROSOL AND SO₂ GAS INTERACT WITH THE STORM SYSTEM AND ARE PARTIALLY SCAVENGED. SO₂ IS ALLOWED TO WET-OXIDIZE IN CLOUDS AND IN RAIN TO FORM SULFATE, USING O₃ AND H₂O₂ AS OXIDANTS. BOTH H₂O₂ AND O₃ ARE ASSUMED TO BE AT SOLUBILITY EQUILIBRIUM IN CLOUD AND RAIN WATER. SO₂ IS AT SOLUBILITY EQUILIBRIUM IN CLOUD WATER, BUT MAY BE AT DISEQUILIBRIUM IN RAIN WATER.

FIRST SET LUMPED PARAMETERS AND STEADY-STATE VARIABLES (GROSS APPROXIMATIONS)

DIMENSION CHAT(16,2)

SO₂ SOLUBILITY (ASSUMED INDEPENDENT OF T, H⁺ AND SO₂ CONC. HERE; GROSS!)

SO₂SOL=4000.

ADJUST STEADY STATES FOR SO₂

$C(IZ,KS02A)=C(IZ,KS02AC)/(1.+SO_2SOL*CLOUD(IZ)*1.8E-5)$
 $C(IZ,KS02C)=C(IZ,KS02AC)-C(IZ,KS02A)$

ACIDITY IN CLOUD AND RAIN (MOLES ACID/LITER WATER)
 THIS IS SIMPLY AN EMPIRICAL CORRELATION WITH SULFATE CONCENTRATION

TABLE A-2 (continued)

```

C      CHAT(IZ,1)=1.864*C(IZ,KS04C)/(CLOUD(IZ)*.018+.0001)+1.4E-5
C      CHAT(IZ,2)=1.864*C(IZ,KS04R)/(RAIN(IZ)*.018+.0001)+1.4E-5
C
C      PARAMETERIZED MASS-TRANSFER COEFFICIENT: SO2 TO RAIN
C
C      PMTC=4.1E-3*RAIN(IZ)**.647
C
C      SO4 NUCLEATION RATE COEFFICIENT (ANOTHER NAIVE APPROXIMATION)
C
C      RNUCL=.1*CLOUD(IZ)
C
C      OZONE AND H2O2 CONCENTRATIONS IN AIR (O3 AND
C      H2O2 ARE ASSUMED CONSTANT HERE TO SIMPLIFY THE
C      EXAMPLE; THIS WILL OBVIOUSLY BE INCORRECT IN THE
C      REAL ATMOSPHERE.)
C
C      C(IZ,KO3A)=5.E-6
C      C(IZ,KH2O2A)=5.E-14
C
C      LOCAL WET-CHEMICAL CONVERSION RATES
C      EQUATIONS ARE SIMPLIFIED VERSIONS FROM PENKETT, AND MARTIN AND DAMSCHEN
C
C      CLOUD:
C
C      CRO3=1.3*C(IZ,KO3A)*C(IZ,KS02C)/SQRT(CHAT(IZ,1))
C
C      CRH2O2=5.5E9*CLOUD(IZ)*C(IZ,KS02A)*C(IZ,KH2O2A)
C
C      RAIN:
C
C      RRO3=1.3*C(IZ,KO3A)*C(IZ,KS02R)/SQRT(CHAT(IZ,2))
C      RRH2O2=7.6E10*C(IZ,KH2O2A)*C(IZ,KS02R)
C
C      NOW CALCULATE THE WET GENERATION RATES (MOLES/M3 SEC)
C
C      WETGEN(KS02AC)=-RIM(IZ)*C(IZ,KS02C)-
+ ACCR(IZ)*C(IZ,KS02C)-CRO3-CRH2O2-AUTO(IZ)*C(IZ,KS02C)
C      WETGEN(KS04C)=-RIM(IZ)*C(IZ,KS04C)-AUTO(IZ)*C(IZ,KS04C)-
+ ACCR(IZ)*C(IZ,KS04C)+CRO3+CRH2O2+RNUCL*C(IZ,KS04A)
C      WETGEN(KS04R)=RIM(IZ)*C(IZ,KS04C)+AUTO(IZ)*C(IZ,KS04C)+
+ ACCR(IZ)*C(IZ,KS04C)+SMEL(IZ)*C(IZ,KS04S)+
+ RRO3+RRH2O2-FREEZ(IZ)*C(IZ,KS04R)
C      WETGEN(KS02R)=PMTTC*(C(IZ,KS02A)-C(IZ,KS02R)/.072)
+ -RRO3-RRH2O2-FREEZ(IZ)*C(IZ,KS02R)+SMEL(IZ)*C(IZ,KS02S)
+ +AUTO(IZ)*C(IZ,KS02C)
C      WETGEN(KS02S)=RIM(IZ)*C(IZ,KS02C)+FREEZ(IZ)*
+ C(IZ,KS02R)-SMEL(IZ)*C(IZ,KS02S)
C      WETGEN(KS04S)=RIM(IZ)*C(IZ,KS04C)+FREEZ(IZ)*
+ C(IZ,KS04R)-SMEL(IZ)*C(IZ,KS04S)
C      WETGEN(KS04A)=-RNUCL*C(IZ,KS04A)
C      RETURN
C      END

```

TABLE A-2 (continued)

```

SUBROUTINE CLEANUP
  INCLUDE 'SCAVCOM.FOR'
  DO 100 IZ=1,NZ
    IF(CLOUD(IZ).EQ.0.) THEN
      C(IZ,KS04A)=C(IZ,KS04A)+C(IZ,KS04C)
      C(IZ,KS04C)=0.
    ENDIF
    IF(SNOW(IZ).EQ.0.) THEN
      C(IZ,KS04R)=C(IZ,KS04R)+C(IZ,KS04S)
      C(IZ,KS02R)=C(IZ,KS02R)+C(IZ,KS02S)
      C(IZ,KS02S)=0.
      C(IZ,KS04S)=0.
    END IF
    IF(RAIN(IZ).EQ.0.) THEN
      C(IZ,KS04A)=C(IZ,KS04A)+C(IZ,KS04R)
      C(IZ,KS02A)=C(IZ,KS02A)+C(IZ,KS02R)
      C(IZ,KS04R)=0.
      C(IZ,KS02R)=0.
    END IF
    JFLAG(IZ)=1
    IF(RAIN(IZ).LE.0..AND.CLOUD(IZ).LE.0..AND.
100 + SNOW(IZ).LE.0.) JFLAG(IZ)=0
    CONTINUE
    RETURN
    END

C
C
C
C
C

SUBROUTINE CLOUDF
  INCLUDE 'SCAVCOM.FOR'

C
C
C
C
CO AND BB CAN BE INTERPRETED PHYSICALLY AS CLOUD(IZ)
AND D(CLOUD(IZ))/DZ AT CLOUD BASE

CC=-(3.*CO+2.*DO*(CT-CB))/(CT-CB)**2
DD=(2.*CO+DO*(CT-CB))/(CT-CB)**3
DO 100 IZ=1,NZ
  CLOUD(IZ)=0.
  IF(Z(IZ).GT.CB.AND.Z(IZ).LT.CT)
+ CLOUD(IZ)=CO+DO*(Z(IZ)-CB)+CC*(Z(IZ)-CB)**2
+ +DD*(Z(IZ)-CB)**3
100 CONTINUE
  RETURN
  END

C
C
C
C
C
C

```

TABLE A-2 (continued)

```

SUBROUTINE SNOWF
  INCLUDE 'SCAVCOM.FOR'
C
C  GENERATES VERTICAL SNOW PROFILES
C

110 IF(FL.LE.CB) GO TO 210
C
C  CASE FOR FREEZING LEVEL ABOVE CLOUD BASE
C
  DO 200 IZ=1,NZ
    SNOW(IZ)=0.
    IF(Z(IZ).LT.CT) THEN
    IF(Z(IZ).GT.FL) THEN
      SNOW(IZ)=DS31*(.5*(CT-CB)**3-1.5*(CT-CB)*(Z(IZ)-CB)**2
      + +(Z(IZ)-CB)**3)
    ELSE
      SNOW(IZ)=DS31*(.5*(CT-CB)**3-1.5*(CT-CB)*(FL-CB)**2
      + +(FL-CB)**3)+CS21*(Z(IZ)-FL)**2
    ENDIF
    SNOW(IZ)=AMAX1(SNOW(IZ),0.)
  END IF
200 CONTINUE
  GO TO 300
C
C  CASE FOR FREEZING LEVEL BELOW CLOUD BASE
C
210 DO 220 IZ=1,NZ
  SNOW(IZ)=0.
  IF(Z(IZ).LT.CT) THEN
  IF(Z(IZ).GT.CB) THEN
    SNOW(IZ)=DS32*(.5*(CT-CB)**3-1.5*(CT-CB)*(Z(IZ)-CB)**2
    + +(Z(IZ)-CB)**3)
  ELSE
    IF(Z(IZ).GT.FL) THEN
      SNOW(IZ)=.5*DS32*(CT-CB)**3+BS12*(Z(IZ)-CB)
    ELSE
      SNOW(IZ)=.5*DS32*(CT-CB)**3+BS12*(FL-CB)+CS22*(Z(IZ)-FL)**2
    ENDIF
  ENDIF
  ENDIF
220 SNOW(IZ)=AMAX1(SNOW(IZ),0.)
300 CONTINUE
  RETURN
  END

```

C
C

TABLE A-2 (continued)

```

SUBROUTINE RAINF
INCLUDE 'SCAVCOM.FOR'

C
C
C
C
C
110  IF(FL.LE.CB) GO TO 210
C
C
C    CASE FOR FREEZING LEVEL ABOVE CLOUD BASE

      DO 200 IZ=1,NZ
      PRECIP(IZ)=0.
      IF(Z(IZ).LT.CT) THEN
      IF(Z(IZ).GT.CB) THEN
      PRECIP(IZ)=DP31*(.5*(CT-CB)**3-1.5*(CT-CB)*(Z(IZ)-CB)**2
+ + (Z(IZ)-CB)**3)
      ELSE
      PRECIP(IZ)=DP31*.5*(CT-CB)**3+CP21*(Z(IZ)-CB)**2
      ENDIF

      ENDIF
200  PRECIP(IZ)=AMAX1(PRECIP(IZ),0.)
      GO TO 300
C
C
C    CASE FOR FREEZING LEVEL BELOW CLOUD BASE
210  DO 220 IZ=1,NZ
      PRECIP(IZ)=0.
      IF(Z(IZ).LT.CT) THEN
      IF(Z(IZ).GT.CB) THEN
      PRECIP(IZ)=DS32*(.5*(CT-CB)**3-1.5*(CT-CB)*
+ (Z(IZ)-CB)**2+(Z(IZ)-CB)**3)
      ELSE
      IF(Z(IZ).GT.FL) THEN
      PRECIP(IZ)=.5*DS32*(CT-CB)**3+BS12*(Z(IZ)-CB)
      ELSE
      PRECIP(IZ)=.5*DS32*(CT-CB)**3+BS12*(FL-CB)+
+ CP22*(Z(IZ)-FL)**2
      ENDIF
      ENDIF
      ENDIF
220  PRECIP(IZ)=AMAX1(PRECIP(IZ),0.)
300  DO 400 IZ=1,NZ
      RAIN(IZ)=PRECIP(IZ)-SNOW(IZ)
      IF(ABS(PRECIP(IZ)).GT.1.E-10)
      + CALL FLUXV(PRECIP(IZ),SNOW(IZ),RAIN(IZ),TEMP(IZ)
      + ,RV,SV,PV)
C

```

TABLE A-2 (continued)

```

C      CONVERT FROM FLUXES TO CONCENTRATIONS
C
      IF(SNOW(IZ).GT.1.E-10) SNOW(IZ)=-SNOW(IZ)/SV
      IF(RAIN(IZ).GT.1.E-10) RAIN(IZ)=-RAIN(IZ)/RV
400    PRECIP(IZ)=RAIN(IZ)+SNOW(IZ)
      RETURN
      END

C
C      SUBROUTINE CBCTFL
      INCLUDE 'SCAVCOM.FOR'

C
C      THIS SUBROUTINE ESTABLISHES THE MSL ELEVATION
C      OF CLOUD BASE, CLOUD TOP, AND FREEZING LEVEL
C      AT HORIZONTAL POSITION IX,IY.

C      THIS VERSION IS A SIMPLIFIED DUMMY SUBROUTINE
C      WHICH IS INTENDED FOR SHAKEDOWN PURPOSES ONLY.
C      ULTIMATELY, WE EXPECT THAT TEMPERATURE-SOUNDING
C      DATA (TEMP(IZ)) WILL BE SUPPLIED BY THE HOST
C      CODE; FOR THE TIME-BEING, HOWEVER, WE SHALL
C      SYNTHESIZE IT AT THIS POINT.

C
C      NOW DUMMY-UP TEMPERATURE PROFILE BY APPLYING
C      PSUEDOADIABATIC LAPSE:

      TEMP(1)=SURFT
      DO 5 IZ=2,NZ
      RHOAIR=CAIR(NZ)*1.E-6
      JFOG=0.
      IF(Z(IZ).GT.CB) JFOG=1
5      TEMP(IZ)=TEMP(IZ-1)
      + +RLAPSE(TEMP(IZ-1),RHOAIR,JFOG)*(Z(IZ)-Z(IZ-1))

C
C      NOW FIND FREEZING LEVEL

C
      IZ=0
      IZ=IZ+1
10     FL=Z(IZ)
      IF(TEMP(IZ).GT.273.2) GO TO 10

C
C      SET INTERNAL PREDICTION PARAMETERS VIA INTERPOLATION
C      OVER LOOK-UP TABLES
C

```

TABLE A-2 (continued)

```

C      CALL INTERP
C
C      NOW SET CLOUD TOP BY CONSTRAINING SYSTEM TO
C      MATCH SURFACE PRECIP RATE
C
C      FIRST SET FUNCTION DESIGNATOR
C
C      IDESIG=1
C      IF(SURFZ.LT.CB.AND.CB.LT.FL) IDESIG=2
C      IF(SURFZ.LT.CB.AND.CB.GT.FL) IDESIG=3
C      IF(SURFZ.LT.FL.AND.CB.GT.FL) IDESIG=4
C
C      NEXT PERFORM NEWTON'S SEARCH FOR CT
C
C      SEQUENTIALLY INCREASE CLOUD THICKNESS UNTIL
C      POSITIVE SURFACE PRECIP IS OBSERVED
C
C      CT1=CB+1000.
50     F1=F(IDESIG,CT1)
C      CT2=CT1+2000.
C      F2=F(IDESIG,CT2)
C      IF(F1.EQ.F2) THEN
C      CT1=CT2+1000.
C      GO TO 50
C      END IF
C
C      SURFACE PRECIP DETECTED; NOW SET UP FOR NEWTON'S SEARCH
C
C      IF(ABS(F1).LT.ABS(F2)) THEN
C      FNEW=F1
C      FOLD=F2
C      CTNEW=CT1
C      CTOLD=CT2
C      ELSE
C      FNEW=F2
C      FOLD=F1
C      CTNEW=CT2
C      CTOLD=CT1
C      END IF
C
C      BEGIN FORMAL NEWTON'S SEARCH
C
C      100  CTSAVE=CTNEW
C      CTNEW=CTOLD-FOLD*(CTNEW-CTOLD)/(FNEW-FOLD)
C      IF(ABS(CTOLD-CTNEW).GT.1.) THEN
C      CTOLD=CTSAVE
C      FOLD=FNEW
C      FNEW=F(IDESIG,CTNEW)
C      GO TO 100
C      END IF
C      CT=CTNEW
C      RETURN
C      END

```

TABLE A-2 (continued)

C
C

FUNCTION RLAPSE(TK,RHOAIR,JFOG)

C
C
C
C
C

ROUTINE FOR CALCULATING LOCAL TEMPERATURE DERIVATIVE
(DT/DZ; DEG K/M) USING DRY OR WET ADIABATS AS
APPROPRIATE. JFOG = 1 WHEN LOCAL CONDENSATION OCCURS.

RLAPSE=-9.76E-3
IF(JFOG.NE.0) THEN
DUMMY1=5.422E3*SAT(TK)/(RHOAIR*TK)
RLAPSE=RLAPSE*(1.+DUMMY1)/(1.+DUMMY1*1.546E3/TK)
END IF
RETURN
END

C
C
C
C
C

FUNCTION SAT(TK)

DIMENSION A(7)

DATA A /6.107799961,4.436518521E-1,1.4289458025E-2,
+ 2.650648471E-4, 3.031240396E-6,2.034080948E-8,
+ 6.136820929E-11/

C
C
C
C
C

ROUTINE FOR CALCULATING THE SATURATION CONCENTRATION OF
WATER VAPOR (GRAM MOLES/CC) AT TK DEGREES KELVIN

TC=TK-273.15
ESAT=A(1)+TC*(A(2)+TC*(A(3)+TC*(A(4)+TC*(A(5)+
+ TC*(A(6)+TC*A(7))))))
SAT=ESAT/(8.3144E4*TK)
RETURN
END

C
C
C
C
C

FUNCTION SSAT(TK)

C
C
C
C
C

SSAT = THE SATURATION CONCENTRATION OF WATER VAPOR OVER ICE
(GRAM MOLES/CM**3) AT TK DEGREES KELVIN
(ESAT IS SATURATION VAPOR PRESSURE IN MB)

TC=TK-273.15
ESAT=6.109177956 + TC*(5.034698970E-1 + TC*(1.886013408E-2
+ TC*(4.176223716E-4 + TC*(5.824720280E-6
+ TC*(4.838803174E-8 + TC*(1.838826904E-10))))))
SSAT=ESAT/(8.3144E4*TK)
RETURN
END

TABLE A-2 (continued)

```

C
C
C
FUNCTION F(IDESIG,CTTEST)
C
C
C
ROUTINE COMPUTES DIFFERENCE BETWEEN
C
C
C
SURFP AND THE COMPUTED SURFACE PRECIP FLUX
C
C
C
CORRESPONDING TO CTTEST, WHICH IS THE
C
C
C
ESTIMATED CLOUD TOP VALUE. USED FOR
C
C
C
NEWTON'S SEARCH FOR CT.

INCLUDE 'SCAVCOM.FOR'
CS31=-1.5*DS31*(CTTEST-CB)
CP31=-1.5*DP31*(CTTEST-CB)
C
GO TO (1,2,3,4), IDESIG
C
CASE FOR SURFZ.GT.CB
C
1
P=CP31*((SURFZ-CB)**2-(CTTEST-CB)**2)+
+ DP31*((SURFZ-CB)**3-(CTTEST-CB)**3)
GO TO 50
C
CASE FOR SURFZ.LT.CB.AND.CB.LT.FL
C
2
P=-CP31*(CTTEST-CB)**2-DP31*(CTTEST-CB)**3
+ CP21*(SURFZ-CB)**2
GO TO 50
C
CASE FOR SURFZ.LT.CB.AND.CB.GT.FL
C
3
P=-CS31*(CTTEST-CB)**2-DS31*(CTTEST-CB)**3
+ BS12*(SURFZ-CB)
GO TO 50
C
CASE FOR SURFZ.LT.FL.AND.CB.GT.FL
C
4
P=-CS31*(CTTEST-CB)**2-DS31*(CTTEST-CB)**3
+ BS12*(FL-CB)+BP22*(SURFZ-FL)
C
50
F=SURFP-P
RETURN
END
C
C

```

TABLE A-2 (continued)

```

C
C
C
  SUBROUTINE INTERP
  INCLUDE 'SCAVCOM.FOR'
C
C  SUBROUTINE INTERPOLATES TO OBTAIN INTERNAL STORM
C  PARAMETERS.
C
C  AT PRESENT THESE ARE SIMPLE POLYNOMIAL FITS, AND
C  THE COEFFICIENTS ARE STATED AS CONSTANTS, RATHER
C  THAN PARAMETERS.
C
C  THE PRESENT PARAMETERS ARE:
C
C  CS31, DS31, CS21, BS12, CP31, DP31, CP21, BP22, CO, DO
C
C  THE FIRST CHARACTER DENOTES TERM IN POLYNOMIAL;
C  I.E.,  $A+B*X+C*X**2+D*X**3$ 
C  THE SECOND DENOTES "SNOW" OR TOTAL "PRECIP"
C  THE THIRD DENOTES ORDER OF FITTING POLYNOMIAL
C  THE FOURTH DENOTES CASE (1 = CB.LT.FL; 2 = CB.GT.FL)
C
  DS31=5.E-12
  CS21=-1.E-7
  BS12=5.E-5
  DP31=5.E-12
  CP21=-1.E-8
  CP22=5.E-4
  CO=.02
  DO=1.E-5
C
C  NOTE: CS32, CP32, CS31 AND CP31 ARE PRESENTLY SET ELSEWHERE VIA CONSTRAIN
TS
  RETURN
  END
C
C
C
C
C
C
C
C
C
C
  SUBROUTINE UDVEL
C
C  STUB FOR FUTURE DEVELOPMENT; NO FUNCTION IN VERSION 1.2
C
  RETURN
  END

```

TABLE A-2 (continued)

C

```

SUBROUTINE SOLAR
  STUB FOR FUTURE DEVELOPMENT; NO FUNCTION IN VERSION 1.2
  RETURN
  END

SUBROUTINE AUTOCON
  INCLUDE 'SCAVCOM.FOR'

  SUBROUTINE CALCULATES PSUEDO FIRST-ORDER RATE
  COEFFICIENT FOR CLOUD AUTOCONVERSION (SEC(-1))
  FOR EACH GRID ELEMENT IZ

    DATA XNC /500./
    DO 100 IZ=1,NZ
      AUTO(IZ)=0.
      IF(CLOUD(IZ).GT.0.) THEN
        DRPMAS=1.8E-5*CLOUD(IZ)/XNC

        DRPMAS= MASS OF AVERAGE CLOUD DROP, GM
        XNC=NO OF CLOUD DROPS/M**3

        IF(DRPMAS.GT.2.348E-9) AUTO(IZ)=9.907E10*
+ CLOUD(IZ)*(DRPMAS**1.667)*(1.-(2.347E9/DRPMAS)**
+ 1.3333)*(1.-(2.040E-9/DRPMAS)**.3333)
        END IF
      CONTINUE
    RETURN
  END

```

TABLE A-2 (continued)

C
C
CSUBROUTINE ACCRET
INCLUDE 'SCAVCOM.FOR'C
C
C
C
C
CSUBROUTINE COMPUTES PSUEDO FIRST-ORDER RATE COEFFICIENT
FOR CLOUD-WATER ACCRETION (SEC(-1)) AT EACH VERTICAL
GRID POINT IZ. CORRESPONDING RATE IS
ACCR(IZ)*CLOUD(IZ) (MOLES CLOUD WATER/M3 TOTAL SPACE SEC)

```

DO 100 IZ=1,NZ
ACCR(IZ)=0.
IF(RAIN(IZ).GT.0..AND.CLOUD(IZ).GT.0.) ACCR(IZ)=
+ 0.0425*RAIN(IZ)**.875
100 CONTINUE
RETURN
END

```

C
C
C
C
CSUBROUTINE RIMING
INCLUDE 'SCAVCOM.FOR'C
C
C
C
C
CSUBROUTINE COMPUTES PSUEDO FIRST-ORDER RATE COEFFICIENTS
FOR CLOUD-WATER RIMING (SEC(-1)) AT EACH VERTICAL
GRID POSITION IZ. CORRESPONDING RATE IS RIM(IZ)*CLOUD(IZ)
(MOLES/M3 TOTAL SPACE SEC)

```

DO 100 IZ=1,NZ
RIM(IZ)=0.
IF(SNOW(IZ).GT.1.E-11.AND.CLOUD(IZ).GT.0.) THEN
TC=TEMP(IZ)-273.15
YOFLAK=5.681E6*EXP(-0.878*AMIN1(TC,0.))
SLAMBD=2.15*(YOFLAK/SNOW(IZ))**.3333
AOLAMB=3.50E-4*SLAMBD
RIM(IZ)=0.319*YOFLAK*(SLAMBD**-3.206)
+ *EXP(-AOLAMB)*(AOLAMB*(AOLAMB+2.))+2.)
END IF
100 CONTINUE
RETURN
END

```

C
C
C

TABLE A-2 (continued)

C
C

```

SUBROUTINE DEPOS
INCLUDE 'SCAVCOM.FOR'

```

C
C
C
C
C
C

```

SUBROUTINE COMPUTES WATER-VAPOR DEPOSITION
RATE TO ICE CRYSTALS, IN MOLES/M3 TOTAL SPACE SEC.
**NOTE** THIS ROUTINE MAY BE BYPASSED UNLESS
PHORETIC OR OTHER DEPOSITION-RELATED SCAVENGING
MECHANISMS ARE INCLUDED IN THE MODEL.

```

```

DO 100 IZ=1,NZ
DEPO(IZ)=0.
TC=TEMP(IZ)-273.15
IF(TC.LT.0..AND.SNOW(IZ).GT.0.) THEN
YOFLAK=5.681E6*EXP(-0.0878*AMIN1(TC,0.))
SLAMBD=2.15*(YOFLAK/SNOW(IZ))**.3333
YCRYST=AMAX1(0.006,400.*((-TC/16.))**.4))
XCRYST=AMAX1(SNOW(IZ)/YCRYST,0.33E-11)
DIFH2O=2.26E-5*((TEMP(IZ)/273.15)**1.81)
GSI=14.76*DIFH2O*(VAPOR(IZ)-1.E6*SSAT(TEMP(IZ)))
DEPCRY=.01089*YCRYST*(XCRYST**.38)*GSI*
+ (1.+.65*XCRYST**.39)
IF(SNOW(IZ).GT.5.E-14) THEN
AOLAMB=AMAX1(0.,ALOG(YOFLAK/(SLAMBD*YCRYST)))
YTFLAK=(YOFLAK/SLAMBD)*EXP(-AOLAMB)
AFLAKE=(1.+AOLAMB)/SLAMBD
DEPO(IZ)=0.349*YTFLAK*AFLAKE*GSI*
+ (1.+374.*AFLAKE*0.75)
END IF
DEPO(IZ)=AMAX1(DEPO(IZ),DEPCRY)
END IF
100 CONTINUE
RETURN
END

```

C
C

TABLE A-2 (continued)

C
C
CSUBROUTINE MELT
INCLUDE 'SCAVCOM.FOR'C
C
C
C
C
CSUBROUTINE COMPUTES PSUEDO FIRST-ORDER RATE
COEFFICIENTS FOR SNOW MELTING
CORRESPONDING RATE IS SMEL(IZ)*SNOW(IZ)
MOLES SNOW/M3 TOTAL SPACE SEC.

```

DO 100 IZ=1,NZ
TC=TEMP(IZ)-273.15
RMELT=TC*(7.46E-4*SNOW(IZ)**.667+1.55E-6*SNOW(IZ)**.868
+1.23E-2*RIM(IZ)*CLOUD(IZ))
RMELT=AMAX1(0.,RMELT)
SMEL(IZ)=RMELT/(SNOW(IZ)+1.E-25)
100 SMEL(IZ)=AMIN1(1.,SMEL(IZ))
RETURN
END

```

C
C
C
C
C
CSUBROUTINE FREEZE
INCLUDE 'SCAVCOM.FOR'C
C
C
C
C
C
CSUBROUTINE COMPUTES PSUEDO FIRST-ORDER RATE
COEFFICIENT (SEC(-1)) FOR ICE FORMATION VIA
RAIN FREEZING
CORRESPONDING RATE IS FREEZ(IZ)*RAIN(IZ)
MOLES RAIN/M3 TOTAL SPACE SEC.

```

DO 100 IZ=1,NZ
FREEZ(IZ)=1.59E-4*YCRYST*C(IZ,KRAIN)**.63
100 FREEZ(IZ)=AMIN1(FREEZ(IZ),1.)
RETURN
END

```

C
C
C

TABLE A-2 (continued)

```

C
C
SUBROUTINE TRNSPT
  INCLUDE 'SCAVCOM.FOR'
  DATA (RVEL(IZ), IZ=1,NZ) /NZ*0./
  DATA (SVEL(IZ), IZ=1,NZ) /NZ*0./
C
C
ROUTINE COMPUTES FALL VELOCITIES (NEGATIVE DOWNWARD)
OF RAIN AND SNOW IN M/SEC UNITS. VARIABLE NAMES ARE
RVEL(IZ) AND SVEL(IZ), WHERE IZ IS THE VERTICAL
GRID INDEX
C
DO 100 IZ=1,NZ
  PRECIP(IZ)=RAIN(IZ)+SNOW(IZ)
  DRAIN(IZ)=3.53*DT*RAIN(IZ)**.25
  DSNOW(IZ)=0.
  RVEL(IZ)=0.
  SVEL(IZ)=0.
  IF(PRECIP(IZ).GT.1.E-5) THEN
    RLAMBD=1149.*PRECIP(IZ)**(-.25)
    AOL=1.02E-3*RLAMBD
    EAOL=EXP(-AOL)
    FACT3=1.+AOL*(1.+(AOL/2.)*(1.+AOL/3.))
    FACT4=1.-EAOL*(FACT3+(AOL**4)/24.)
    FACT3=1.-EAOL*FACT3
    FACT34=SQRT(FACT3*FACT4)
    RVEL(IZ)=-(1.-FACT34)*252.2/SQRT(RLAMBD)-
+ 16220.*FACT4/RLAMBD
    END IF
    IF(SNOW(IZ).GT.1.E-5) THEN
      TC=TEMP(IZ)-273.15
      YOFLAK=5.681E6*EXP(-0.0878*AMIN1(TC,0.))
      SLAMBD=2.148*(YOFLAK/PRECIP(IZ))**0.3333
      AFLAKE=1./SLAMBD
      SVEL(IZ)=-4.06*AFLAKE**.206
      VBARG=.00156*AFLAKE**.206
      IF(AFLAKE.LT.3.37E-4) SVEL(IZ)=-1296.*AFLAKE**.927
      IF(AFLAKE.LT.4.6E-5) VBARG=6.95*AFLAKE**.927
      DSNOW(IZ)=DT*VBARG*VBARG
    END IF
100 IF(PRECIP(IZ).GT.0.)RVEL(IZ)=
+ RVEL(IZ)*RAIN(IZ)/PRECIP(IZ)+
+ SVEL(IZ)*SNOW(IZ)/PRECIP(IZ)
  RETURN
END
C
C
C
C

```

TABLE A-2 (continued)

```

C
C
C
C
C
C
C
C
C
SUBROUTINE COVER(IFLAG)
C
C
C
STUB FOR FUTURE DEVELOPMENT; NO OPERATION IS VERSION 1.2
RETURN
END
C
C
C
C
C
C
SUBROUTINE EVAPOR
INCLUDE 'SCAVCOM.FOR'
C
C
C
SUBROUTINE COMPUTES RAIN EVAPORATION RATES
(MOLES/M**3SEC). **NOTE** THIS SUBROUTINE MAY BE
C
C
C
BYPASSED UNLESS PHORETIC OR OTHER EVAPORATION-DEPENDENT
SCAVENGING MECHANISMS ARE MODELED.
C
DO 100 IZ=1,NZ
EVAP(IZ)=0.
IF(CLOUD(IZ).LE.0..AND.RAIN(IZ).GT.0.) THEN
EVAP(IZ)=3.56E-3*(1.E-6*SAT(TEMP(IZ))-VAPOR(IZ))
+ *RAIN(IZ)**.65
EVAP(IZ)=AMAX1(0.,EVAP(IZ))
END IF
100 CONTINUE
RETURN
END
C
C
C
C
C
C

```

TABLE A-2 (continued)

C
C
C
C
C
C

SUBROUTINE FLUXV(P,S,R,T,RV,SV,PV)
 DIMENSION BASE(20),RVBASE(20),SVBASE(6,20)

INTERPOLATION ROUTINE FOR RAPID CALCULATION OF PRECIP AND SNOW
 VELOCITIES FROM BASE DATA OBTAINED FROM PLUVIUS.

SET INTERPOLATION TABLES

DATA(BASE(I),I=1,20) /0.,5.309E-7,2.096E-6,6.045E-6,1.567E-5,3.885E-5,
 + 9.432E-5,2.266E-4,5.398E-4,1.274E-3,2.970E-3,6.829E-3,.01550,
 + .03476,.07726,.1705,.3747,.8207,1.794,3.918/
 DATA(RVBASE(I),I=1,20) /0.,.5309,.6987,.8635,1.045,1.253,1.497,1.784,
 + 2.117,2.493,2.903,3.336,3.785,4.244,4.716,5.205,5.717,
 + 6.261,6.844,7.474/
 DATA (SVBASE(1,I), I=1,20)/0.0000E+00,0.1354E0,0.1877E0,0.2417E0,
 +0.3030E+00,0.3754E+00,0.4626E+00,0.5687E+00,0.7031E+00,0.7986E+00,
 +0.8468E+00,0.8940E+00,0.9430E+00,0.9925E+00,0.1044E+01,0.1098E+01,
 +0.1155E+01,0.1214E+01,0.1277E+01,0.1343E+01/
 DATA (SVBASE(2,I), I=1,20)/0.0000E+00,0.1098E0,0.1537E0,0.1983E0,
 +0.2485E+00,0.3078E+00,0.3791E+00,0.4656E+00,0.5707E+00,0.7002E+00,
 +0.7955E+00,0.8455E+00,0.8907E+00,0.9375E+00,0.9865E+00,0.1038E+01,
 +0.1089E+01,0.1174E+01,0.1277E+01,0.1343E+01/
 DATA (SVBASE(3,I), I=1,20)/0.0000E+00,0.8985E-1,0.1248E0,0.1598E0,
 +0.2001E+00,0.2479E+00,0.3059E+00,0.3765E+00,0.4626E+00,0.5680E+00,
 +0.6936E+00,0.7988E+00,0.8413E+00,0.8858E+00,0.9321E+00,0.9806E+00,
 +0.1028E+01,0.1141E+01,0.1277E+01,0.1343E+01/
 DATA (SVBASE(4,I), I=1,20)/0.0000E+00,0.7370E-1,0.1009E0,0.1297E0,
 +0.1625E+00,0.2013E+00,0.2481E+00,0.3051E+00,0.3745E+00,0.4586E+00,
 +0.5608E+00,0.6835E+00,0.7949E+00,0.8369E+00,0.8809E+00,0.9268E+00,
 +0.9704E+00,0.1113E+01,0.1277E+01,0.1343E+01/
 DATA (SVBASE(5,I), I=1,20)/0.0000E+00,0.5931E-1,0.8223E1,0.1060E0,
 +0.1329E+00,0.1647E+00,0.2029E+00,0.2492E+00,0.3056E+00,0.3738E+00,
 +0.4558E+00,0.5543E+00,0.6768E+00,0.7817E+00,0.8325E+00,0.8760E+00,
 +0.9166E+00,0.1090E+01,0.1277E+01,0.1343E+01/
 DATA (SVBASE(6,I), I=1,20)/0.0000E+00,0.4815E-1,0.6746E1,0.8612E1,
 +0.1077E+00,0.1335E+00,0.1647E+00,0.2028E+00,0.2493E+00,0.3060E+00,
 +0.3734E+00,0.4533E+00,0.5486E+00,0.6652E+00,0.7684E+00,0.8281E+00,
 +0.8664E+00,0.1070E+01,0.1277E+01,0.1343E+01/
 TC=T-273.2

C
C
C

DO TOTAL PRECIP CALCULATIONS

10

RV=0.
 IF (ABS(R).GT.1.E-10) THEN
 N=1
 N=N+1
 IF(ABS(R).GT.BASE(N)) GO TO 10
 RV=RVBASE(N-1)-(RVBASE(N)-RVBASE(N-1))*R/(BASE(N)-BASE(N-1))
 RV=-RV
 END IF

TABLE A-2 (continued)

```
C
C DO SNOW CALCULATIONS
C
SV=0.
IF(ABS(S).GT.1.E-10) THEN
M=1
20 M=M+1
IF (ABS(S).GT.BASE(M)) GO TO 20
N=-TC/10+1
M=MAX0(1,M-1)
N=MAX0(1,N)
QQ=-TC/10.-MM
PP=(S-BASE(M))/(BASE(M+1)-BASE(M))
SV=(1.-PP-QQ)*SVBASE(N,M)+PP*SVBASE(N,M+1)+QQ*SVBASE(N+1,M)
END IF
C
C MODIFY TOTAL PRECIP CALC. FOR MIXED RAIN AND SNOW, AND
C CONVERT SIGNS TO NEGATIVES (DOWNWARD FALL VELOCITIES)
C
IF(P.GT.1.E-10) PV=(R*RV+S*SV)/P
SV=-SV
RETURN
END
```